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#### BACKGROUND MATERIAL FOR LECTURES BY

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# **Physics of Fracture**

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### i. Introduction

Thirty years before the date of this article, one of the founding editors of this series proposed and elaborated the concept of the imperfection in a nearly perfect solid<sup>1</sup> as a way of understanding the structure-sensitive properties of crystalline matter. His synthesis has since proven to be one of the bases upon which much of modern materials science rests. Included in the original list of fundamental imperfections was the dislocation, which was originally proposed by Orowan *et al.* in  $1934^{2-4}$  to explain the plastic mechanical properties of a solid. We suggest that the crack should be added to this list, and argue that the crack and dislocation taken together comprise what might be termed a "complete set" for understanding the mechanical failure of crystalline materials.

The argument follows from the fact that materials failure exhibits a bipolar character; i.e., materials are classifiable in terms of their relative brittleness or ductility. A material at the extreme ductile pole flows plastically like taffy when stressed above its elastic limit, and finally separates by necking, as depicted in Fig. 1. Pure copper single crystals are excellent prototypes of this extreme pole. The necking failure in this crystalline case involves only dislocation processes, and is often termed plastic rupture. At the opposite pole of brittle failure, the material is perfectly elastic up to a critical stress at which it cleaves catastrophically (Fig. 2). Ordinary silicate glasses are the most widely known examples of brittle fracture, but, because it is crystalline, silicon at room temperature is perhaps a better prototype. At this pole, no dislocation activity

<sup>1</sup> F. Seitz, in "Imperfections in a Nearly Perfect Solid" (R. Smoluchowski, ed.), p. 3. Wiley, New York, 1952.

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Fig. 1. A rod of ideally ductile material when pulled develops a region of plastic instability which finally thins uniformly down to a sharp point.





at all is observable at failure, and the fracture is due to the propagation of a single atomically sharp cleavage crack right through the specimen.

The conceptual importance of the two types of defects operating at these opposite poles derives from the fact that the material in each case fails at an average stress level which is often many orders of magnitude less than the theoretical strength of the material, expressed in terms of its constituent atomic bonds. This low failure stress at the two polar extremes thus constitutes a fundamental problem in mechanical failure. The reader is reminded that, in the case of the dislocation, this problem is solved in principle, because the dislocation is a lattice defect whose atomically sized core contains stresses equal to the theoretical shear strength of the constituent atomic bonds. Under a modest external stress, the dislocation translates through the crystal, shearing bonds as it goes, in a progressive fashion. When it traverses a crystal from one side to another, a shear of one atom spacing results. Generation of new dislocations in the local region of the macroscopic neck in the sample then

<sup>&</sup>lt;sup>2</sup> E. Orowan, Z. Phys. 89, 605, 634 (1934).

<sup>&</sup>lt;sup>3</sup> M. Polanyi, Z. Phys. **89**, 660 (1934).

<sup>&</sup>lt;sup>4</sup> G. I. Taylor, Proc. R. Soc. London Ser. A 145, 362 (1934).

explains its final separation. Similarly, the atomically sharp cleavage xrack (Fig. 3) possesses a core of atomic size at its tip where the stresses are magnified to the tensile strength of the bonds, and when the crack passes through the crystal, again the bonds are broken progressively until the entire crystal cleaves into two halves. Thus the dislocation and crack are twin lattice defects which jointly provide an answer to this first fundamental problem of materials failure.

Fortunately for materials technology, however, the vast majority of materials are situated at neither pole, and are much stronger than pure single crystal copper, and much tougher than untreated silicate glass. (The concept of "toughness" will be defined more carefully later, but for the present it can be taken as simply the energy absorbed from the external stressing machine as the crack propagates.)

Materials of high strength and toughness have been the goals for allarge portion of materials research for many years, and the detailed understanding of these properties is still elusive. Qualitatively, however, materials are tough and strong because of the rich variety of interactions dislocations have with themselves, with cracks, and with other imperfections, and perhaps the greatest conceptual difficulty of the subject is connected with the collective character of this interaction. Thus the understanding of the two complementary material properties of strength and toughness constitutes a second major fundamental problem in materials science of very great proportion, which is yet largely unsolved. In this article, we shall be primarily concerned with toughness and the properties of cracks, which constitutes only half of the:total problem associated with mechanical failure, though the problem of strength is closely related to and overlaps that of toughness.

It is possible to get close to the heart of the problem of toughness by focusing on the structure of the underlying cracks in a solid. In the next section, where some of the background phenomenology of fracture will be

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FIG. 3. Diagram of a crack in a two-dimensional square lattice with external forces exerted at the center of the crack. Bonds at the two crack tips are nonlinear. The nonlinear attractive forces at the tip are labeled f and the external applied forces at the center of the crack are labeled  $\tilde{F}$ .

inlisplayed, the ductile/brittle duality will be found to extend or persist well into the middle ground of the ductile/brittle axis. It persists in the sense that even though a failure may appear macroscopically to be cracklike, on closer m croscopic examination, the "crack" will be found to be quite blunt and integular in shape, without the characteristic atomically sharp tip of the theavage crack. On the other hand, a crack showing considerable toughness may consist of a sharp underlying cleavage crack, but be associated with large numbers of dislocations. On moving from relatively ductile to relatively brittle materials, the shape of the underlying crack changes from a blunt notch or recunded hole which expands by purely plastic means (i.e., dislocation Normation from the material ahead of the crack, or from corners on the crack surface, either of which usually leads to necking on a microscale) to a sharp prack which advances by cleavage. This change in mechanism when induced in s given specimen or structure usually has dramatic, tangible, and even practical consequences, as for example when a material becomes embrittled by external chemical attack.

A valuable key in the approach to the toughness problem is to distinguish thetween an intrinsically brittle material and an intrinsically ductile one in literms of the atomic structure of their cracks. We show that the first class of imaterials can sustain an atomically sharp crack stably in the lattice without lbreakdown by dislocation generation, while the second class cannot. In those imaterials where the sharp crack is stable, cleavage crack growth is possible; in ithe opposite case, only tougher ductile crack growth is possible. This it is inction between intrinsic brittle or ductile cracks may depend upon texternal conditions, as well as on the material itself. This distinction will be imodified as we develop it, for example, by considering a middle ground where ithe crack is only barely stable, and by considering the effects of dislocations generated in the bulk material; but without undercutting its overall usefulness in sorting out the enormously complex phenomenology of fracture.

After establishing the basic distinction between intrinsically ductile and intrinsically brittle materials, the study of toughness then proceeds to develop the dislocation interactions with the two types of cracks and from this to establish the fracture criterion. Unfortunately, much of this analysis, especially for ductile cracks, still remains to be done, and even in the case of the brittle crack, is only in semiquantitative form. But the central role of the istructure of cracks also emphasizes a familiar type of problem to physicists, mamely the atomic structure of defects. In the case of the crack, the severe mature of the distortion of the lattice by the defect puts the quantitative study of the structure of cracks still largely in the "research to be done" category. The previous paragraph is couched in theoretical terms. But the science of fracture at the time of writing is entering a period of intense development on the experimental side as well, which is generating a theory-experiment

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confrontation and consequent flowering of our understanding, reminiscent of the period 1955–1965 in dislocation research. This experimental development has largely been due to the work by Hockey in brittle materials, and Ohr, Wilsdorf, Neuman, their co-workers, and others in ductile materials; usually working with thin films in electron microscopes. In a sense, then, this article is able to point to some guiding principles, and initial theoretical and experimental findings whose major purpose will be to point with hope toward the future.

In an article like this, it will be necessary to establish some background information. Therefore, in the next section, a series of microphotographs will be presented to provide the reader with a necessary observational perspective. In Part III, the required results from the elastic analysis of cracks and dislocations will be presented. In Part IV, a central theorem of Eshelby on the force exerted on elastic singularities will be used to derive the forces on cracks and dislocations and the interactions between them. Then, in Parts V and VI, the central theme of the structure and properties of sharp cracks in lattices, including interactions with external chemical environments, will be addressed. In Part VII, the idea of dislocation shielding of static and moving cracks is presented along with the simple available models for fracture toughness and the available experimental evidence.

We shall not attempt to cover the more applied aspects of fracture, partly because it would be unsuitable in an article emphasizing the physical fundamentals of fracture, but also because the more important applications still await an adequate description in terms of fundamental ideas. Hydrogen embrittlement and fatigue crack initiation are just two examples where a final description is probably still well in the future, even though some of the fundamental tools are coming to hand. Nor shall we have space to consider fracture in polymers, where the effects of crazing bring up a different set of phenomena that are now being successfully tackled.

Finally, we note here that the subject of fracture is one involving a number of disciplines. We shall, of course, repeatedly delve into physics, chemistry, and materials science. However, fracture science also deeply involves continuum mechanics. The reason is easily seen from inspection of Fig. 3: A crack requires an external force for its existence. If this force disappears, in principle the lattice will simply heal itself. Hence, the manner in which this force manifests itself at the crack tip is a continuum mechanics problem that will involve the way the force is applied to the external surfaces of the body, and may involve sophisticated mathematical descriptions of deforming media. Fortunately, we shall find it possible to condense most of the mechanical aspects of the problem into a local parameter at the crack tip called the local stress intensity factor. However, the reader should be aware that there are classes of problems such as propagation of cracks through plastic media, or the role of plastic instability in the propagation of ductile fracture, where continuum plasticity approaches must be used.

### **N. Observational Background and Initial Concepts**

A casual observation of the fracture of any practically useful engineering material shows a very complex phenomenon. This section will thus be devoted to a demonstration of some of this complexity, and will also demonstrate the observational basis for the scientific approach which we have outlined in the Introduction, but which must be firmly established on an observational basis. At the same time, the reader will appreciate from a perusal of the fractographs which we will display here the limitations of making quantitative predictions of fracture toughness for engineering materials.

## 1. MACROSCOPIC FRACTOGRAPHIC OBSERVATIONS

Before displaying the rather sobering complexity which we have alluded to above, Fig.  $4^5$  illustrates the beautifully symmetric brittle fractures which are possible in a material such as glass. The figure shows a hertzian crack with cylindrical symmetry produced by an indentation at one point on the surface of the glass. The fact that the glass is completely isotropic results in a highly symmetric fracture mode and a highly regular overall configuration. A BB pellet stopped by ordinary plate glass will display such a hertzian crack. At the opposite extreme, Fig.  $5^6$  illustrates the chisel point which is formed when a highly ductile metal is pulled to ultimate fracture. Each of these two examples is of course a direct illustration of the two poles of fracture shown schematically in Figs. 1 and 2 of the Introduction.



Fig. 4. A Herizian crack produced in the upper surface of a block of glass by a round indenter (after Roesler<sup>3</sup>).

<sup>5</sup> F. C. Rocsler, Proc. Phys. Soc. B 69, 981 (1956). <sup>6</sup> H. G. F. Wilsdorf, Mater. Sci. Eng. 59, 1 (1983). 7

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Fig. 5. A chisel point formed in a rod specimen of gold after necking and rupture. Original specimen was 0.15 cm in diameter (courtesy of H. Wilsdorf<sup>6</sup>).

# 2. MICROSCOPIC OBSERVATIONS

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On a microscopic level the rough surface typical of a high-toughness metal still displays a high complexity. The surface is highly dimpled on a micrometer level and below, as shown in Fig. 6. These dimples have been shown to be caused by the formation of holes which form ahead of a main crack as shown in Fig. 7. As the crack grows, the holes enlarge by plastic means and coalesce with the main crack and with other holes in the vicinity. In these cases the growth and coalescence of the voids with the main crack are really a manifestation of the necking process on a microscale. As shown in Fig. 6, the larger voids are found to be nucleated at the site of precipitated particles in the



FIG. 6. Ductile fracture surface, showing the final dimpled structure of hole growth. Precipitate particles are visible in some of the dimples which served as nucleation sites for the holes (courtesy of C. Internance).



FIG. 7. Schematic drawing of the development of a ductile fracture from a blunt crack embedded in a material containing inclusions. Microcracks are nucleated at the inclusions, which are blunted in turn. (COD is an abbreviation for crack opening displacement.)

matrix. The precipitate particles may fail on their interface with the matrix, or brittle precipitates may cleave. In either case, they are left behind in the holes, as shown in Fig. 6.

In a brittle ceramic, or in a steel in an embrittled condition (such as when under hydrogen or other chemical attack, or when the temperature is low and the strain rate high), the fracture morphology is different. Figure 8<sup>7</sup> shows an intergranular brittle fracture in which the crack proceeds without any obvious void formation, and a very clean form of separation at the grain boundaries occurs. Transgranular brittle fracture can also occur, often mixed with the intergranular variety. This example shows how important the metallurgical and ceramic microstructural variables such as grain-boundary segregation and second-phase coarsening are to fracture toughness.

### 3. PROTOTYPE FRACTURES

In the next set of observations, the phenomena characteristic of more ideal conditions are illustrated. Figure 9 shows the results of Hockey<sup>8</sup> for cracks in silicon. Figure 9a shows a completely brittle cleavage crack at low temper-



FIG. 8. Brittle crack in a ceramic.<sup>7</sup> The crack has opened along the grain boundaries of the material, giving rise to a very irregular morphology. Such forms of brittle fracture are also observed in metals.

atures in which no dislocation activity is observable. Figure 9b shows that the cracks in silicon are nearly completely reversible. This crack presumably has grown beyond its final position, with a network of misfit dislocations appearing between the initial and final positions of the crack after regression has occurred. Figure 9c shows a crack grown in silicon above the ductile transition temperature, in which significant dislocation activity in the presence of the crack tip is visible. It is not clear whether these dislocations are formed out of the crack after it stops, or whether they have been carried along by the crack from the deformation zone in which the crack itself was formed. Figure 10 shows the electron channeling pattern of a transgranular cleavage surface in embrittled steel, which illustrates that dislocations are generally present even in very brittle fracture in steels, except at high crack speed.

Figure 11<sup>9</sup> shows the crack configuration of iron-2.6 at.% silicon. The crack is wedge-shaped just as one would expect if dislocations were emitted on

\* H. Vehoff and P. Neumann, Acta Metall. 28, 265 (1980).

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<sup>&</sup>lt;sup>1</sup> E. Fuller, unpublished photograph of a crack in Si<sub>2</sub>N<sub>4</sub> at high temperature.

<sup>\*</sup> B. Lawn, B. Hockey, and S. Wiederhorn, J. Mater. Sci. 15, 1207 (1980).



Fig. 9. (a) An electron microscograph of a fully brittle crack in Si. In the photograph, the crack is seen edge on. In (b) a brittle crack has regressed from its initial position, leaving a network of misfit dislocations on the closed portion of the cleavage plane. (c) Cracks formed in Si at 500 °C are associated with dislocations as shown (see Lawn *et al.*<sup>4</sup>). (Courtesy of B. Hockey.)



FIG. 9. (Continued).

slip planes intersecting the crack tip (see also Fig. 43). In this case the material "slides off" on its slip plane which is at an oblique angle to the plane of the crack. When hydrogen is introduced into the system (Fig. 11a) the angle is made more acute, showing that cleavage and emission take place simultaneously.

Figure 12 shows the experimental configuration used by Ohr and coworkers.<sup>10</sup> When a region in the very thin section near the hole is imaged in the microscope, the results are shown in Fig. 13.<sup>11</sup> In this case the crack spews out screw dislocations on its cleavage plane. The crack has a substantial region near its tip (termed an elastic enclave or dislocation free zone) where no dislocations are present. Similar experiments have been performed in a variety of other metals (see Table I).

A more typical form of purely ductile failure is shown in Fig. 14,<sup>12</sup> where experiments performed by Wilsdorf,<sup>6</sup> again in thin foils, exhibit a more normal

11 S. Kobayashi and S. Ohr, Scripta Metall. 15, 343 (1981).

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12 R. Lyles and H. G. F. Wilsdorf, Acta Metall. 23, 269 (1975).

<sup>&</sup>lt;sup>10</sup> S. Ohr, J. Horton, and S. Chang, in "Defects, Fracture, and Fatigue." (G. C. Sih and J. W. Provan, eds.), p. 3. Nijhoff, The Hague, 1983.



FIG. 10. Electron channeling patterns from portions of a cleavage crack in hydrogen embrittled steel. A blurred pattern indicates lattice plane rotations caused by presence of dislocations. In the figure, the crack accelerates from its initial position at rest in the region of pattern 1 to a high velocity near pattern 6. At the high velocity (an appreciable fraction of the sound velocity), there is no measurable increase in the dislocation density above that of the initial material. (Courtesy of W. Gerberich and K. A. Peterson.)

failure by hole growth and coalescence. The event shown in the figure is the final result of the chisel necking shown in Fig. 5. In this case the foil thins by plastic processes and small holes form in the dislocation cell walls, which then grow to a size equal to the film thickness and the large holes shown in the figure then become visible. These holes are crystallographic in shape corresponding to the slip planes in the material. A mixed form of growth seems to take place in which some dislocations are emitted from the crack tip itself, while others are generated at sources in the medium very close to the crack tip. Although these films are very thin, the hole formation and growth processes illustrated





FIG. 11. In (a) sharp cracks are formed in a hydrogen atmosphere in Fe (+ Si). In (b) the crack opens entirely by dislocation slide-off at the crack tip. In both cases, dislocations are emitted from the crack tip, and form slip bands. In (a), cleavage must also be present. The angle of the wedge opening in (b) is defined by the intersection angle of the two slip planes with the crack plane (after Vehoff and Newmann<sup>9</sup>).

are thought to be analogous to those taking place in bulk samples such as in Figs. 6 and 7. In Fig. 14, of course, the void generation takes place in the dislocation cell walls rather than at precipitate particles, perhaps corresponding to the smaller holes formed in Fig. 6. It is in fact generally observed on close examination that the large voids formed at large precipitated second-phase particles are often connected by void sheets composed of very small voids, and the question of whether these sheets are created at small precipitates or are generated at dislocation cell boundaries has not been fully sorted out.<sup>6,13</sup>

43 A. Thompson and P. Weirauch, Scripta Metall. 10, 205 (1976).

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FIG. 12. Specimen geometry used in electron microscope fracture experiments by Ohr and coworkers.<sup>10</sup> The crack grows out of the thinned region nearest the hole in the center.





Fig. 13. (a) Dislocations emitted from the tip of a crack in a foil of copper. The crack has grown from the left. Immediately ahead of the crack is a region free of dislocations. The pile-up of dislocation= is seen extending on the cleavage-slip plane to the right. In (b) the crack dislocation geometrica configuration is illustrated (after Kobayashi and Ohr<sup>14</sup>).



FIG. 14. Side view of a growing fracture in a thin film of gold. Holes are shown nucleating ahead of the crack (see Lyles and Wilsdorf<sup>12</sup>). (Courtesy of H. G. F. Wilsdorf.)

## 4. FRACTURE MODE AND CRACK DISLOCATIONS

The previous fractographs indicate that real cracks are three-dimensional defects whose fracture planes may be very rough surfaces, that even brittle fractures may take place on the three-dimensional network of a grain boundary structure, and that interaction with various kinds of imperfections in a material is common. Nevertheless, for analytical purposes, it is desirable to idealize a crack line as a one-dimensional line defect on a flat cleavage plane. There are, then, three modes of cracks corresponding to the different orientations of the external stress with respect to the fracture plane. These three modes are analogous to the two different classes of dislocations: screw and edge. In the case of the crack, a cut is made in the medium which becomes the cleavage plane, and simple shear or tensile stresses are exerted on the external surfaces of the specimen. In Mode I the stress is a tensile stress with principal axis normal to the cleavage plane, as shown in Fig. 15a. This mode is the only one leading to physical fracture, because, unless the external stress physically separates the two surfaces on the cleavage plane, then rewelding would occur even after the stress is applied. In Mode II the stress is a shear parallel to the cut in the x, direction (we use the coordinate system of Fig. 16a). In Mode III the stress is a shear parallel to the cut in the antiplane or  $x_1$ direction. Mode III is important because antiplane strain is associated with a particularly simple analysis, and we shall make extensive use of this analysis in order to describe results for cracks in a generic sense. Even in the case of simple two-dimensional cracks, mixed cases are common. For example, a crack may be produced which is primarily Mode II or III, but with enough Mode I present to separate the cleavage plane.

We note here an idea originally proposed by Friedel<sup>14</sup> that the displacement on the cleavage plane of a crack may be represented by a distribution of dislocations of appropriate Burgers vector. Such a representation can be used analytically to describe the stress field of a cleavage crack (see Part III).

# 5. THE OBSERVATIONAL BASIS FOR FRACTURE SCIENCE

From the selected illustrations above, an observational basis can be constructed for our approach to fracture, as follows.

(a) In practice, cracks are most often flaws of a complex three-dimensional form which sometimes only vaguely approximate the three idealized modes of



Fig. 15. The three modes of fracture. In each case, the crack is formed by making a planar slit in the material, with the crack line along the edge of the cut. In Mode I, the opening mode, the force is exerted normal to the cleavage plane. In Mode II, the force is in the plane of the crack normal to the crack line. In Mode II, the force is in the plane of the crack normal to the crack line. In Mode II, the force is in the plane of the crack line. Modes II and III are shear cracks.

Fig. 15. However, because of the necessity of developing models which can be analyzed and described in accessible mathematics, we are led to the study of these idealized modes.

(b) In some solids, the crack is capable of cleavage advance without intrinsic generation of dislocations (Fig. 9). (By intrinsic is meant generation from the crack tip itself, independent of external sources.) In others, when the crack is stressed, dislocations are emitted from the tip without cleavage (Figs. 11 and 13). Crack advance in the second case takes place by ledge formation or slide-off at the crack tip, Fig. 11. The shape of the crack in the cleavage case is atomically sharp at its tip (Fig. 9). When the crack advance is controlled entirely by dislocation emission, the shape is that of a wedge whose opening angle is equal to the angle between the operating slip planes (Fig. 11; see also Fig. 43).

(c) The ubiquitous presence of dislocation sources in nearly all materials and the stress concentration around the crack tip assures that dislocations, sometimes in copious numbers, are generated which accompany the fracture process (Figs. 9 and 10). Only in exceptional cases, such as in Si at low temperatures, or in fast fracture when the crack outruns its dislocation cloud, are ideal brittle fractures observed. Since dislocations and cracks are singularities in an elastic medium (if the crack tip has a sharp angle), their stress fields give rise to strong crack-dislocation interactions which play a central role in determining the overall toughness.

(d) The effect of plasticity external to the crack is to blunt the crack by means of the steps formed on the cleavage surfaces when dislocations are annihilated there. The final macroscopic shape of the crack blunted by dislocation absorption will be determined by the combined effect of the available slip systems, stress distribution around the crack, the characteristics of the sources such as operating stress, etc., and the mobility and mean free

<sup>&</sup>lt;sup>14</sup> J. Friedel, "Les Dislocations," p. 214. Gauthier-Villars, Paris, 1956; "Dislocations," p. 320. Pergamon, London, 1964. See also B. A. Bilby and J. D. Eshelby, in "Fracture" (H. Liebowitz, ed.), Chap. 1, p. 99. Academic Press, New York, 1968.

path of the dislocations. A variety of final shapes is thus possible, but in general the shape of the crack will not be dominated by crystallographic features as in the case for the cleaving or emitting crack. Further, such a crack (we shall often refer to blunted cracks as notches), of itself, will not advance solely by dislocation absorption under continued stressing, but will simply increase its effective radius at the tip by indefinite plastic blunting. In practice, however, inhomogeneities in the material cause microcracking to occur ahead of the main crack with subsequent hole growth (Fig. 7). Blunting bli the main crack stops when a void is absorbed, and "crack" advance takes place by accretion of the voids to the main crack. The void formation and accretion also limit the necessary region of plastic activity to that surrounding the blunted crack tip; so that fracture can occur without raising the stress of the entire specimen to the plastic yield value.

We are thus led to propose three prototype cracks: cracks which cleave, cracks which emit dislocations, and plastically blunted notches which merely activate external plastic flow in the surrounding medium. The physical mechanisms in each case are quite distinct, and each type tends to correspond to a particular geometry. Mixed cases are to be expected, however. Thus, external dislocation sources usually are activated by cleavage cracks, even though the crack advances by cleavage and no hole growth is observed (Figs. 9c and 10). Likewise, in cases where the fracture is predominantly by plastic hole growth, significant portions of transgranular or grain boundary cleavage facets may be observable in the fractured surfaces. Also the initial stages of hole formation normally involve cleavage, and the whole question of how the cleavage (or emission) events are affected by the alteration of crack shape caused by dislocation absorption is unanswered. Finally, i mixed cleavage-emission is possible in cases where a crack is balanced on the borderline between cleavage and emission (Fig. 11a).

The correlation between these three prototype cracks, which are diassified according to their atomic structures and the mechanisms of their advance, with the overall fracture toughness and the brittle/ductile polarity, becomes the central task of fracture science. Qualitatively, the brittle pole is associated with the cleavage crack, while the emitting crack and the plastically/blunted crack are forms of ductile fracture.

The crucial physical implication of this line of thought is that the structure of the underlying crack and its immediate environment determines the overall mechanical response. The atomic structure of the tip will dictate whether the crack is a cleaver or an emitter, and the properties of the dislocations and their sources in the medium and their interactions with the crack will determine whether the core crack can ever be stressed sufficiently so that cleawage or emission is possible. Thus, the balance achieved regarding the brittle/ductile polarity in any fracture event is determined partly by the bonding of the atoms of the solid, partly by the lattice structure, partly by the microstructure of the material, and partly by the external environment. A material may change from ductile hole gowth to brittle cleavage by modifying these factors in various ways. For example, for any given material, a variety of chemical species can be embrittling agents. Hydrogen in steels and water in glass are examples. Toughness is also a function of strain rate and temperature, and steels typ:cally undergo a dramatic ductile-to-brittle transition along the axes of types parameters.

# III. The Elastic Fields of Cracks and Dislocations

### 6. INTRODUCTION

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Many scientists view elasticity as a field essentially completed by the end of the 19th century. However, in this article the mathematics of elasticity will play a much more important role than that of an ancient formalism to be priefly revisited. Rather, cracks and dislocations, viewed as interacting singularities in the elastic field, will lead to new insights into the toughness of materials, and much of the mathematics required will be unfamiliar to most readers with a nodding acquaintance with the elements of classical elasticity. For full-scale numerical calculations in a particular crystal, anisotropic elasticity is the mode of choice, and a brief review of some aspects of amisotropic theory will be given. However, we shall find the more analytic results possible in isotropic theory to be more useful in this article for developing the physical insight which is our main purpose.

The basic reference for this section is the treatise on elasticity by Muskhelishvili<sup>13</sup> because it contains an authoritative treatment of twodimensional elasticity, complex potentials, conformal mapping, and Muskhelishvili singular integrals. However, it does not address cracks or fracture problems. For collateral reading on fracture, the reader is referred to the excellent articles by Bilby and Eshelby,<sup>16</sup> Rice,<sup>17</sup> Sih and Libowitz,<sup>18</sup>

<sup>&</sup>lt;sup>13</sup> N. Muskhelishvili, "Some Basic Problems in Mathematical Theory of Elasticity." Noordhoff, Levden, 1977.

<sup>&</sup>lt;sup>14</sup> B. Bilby and J. Eshelby, in "Fracture" (H. Liebowitz, ed.), Chap. 1, p. 99. Academic Press, New York, 1968.

<sup>15</sup> J. Rice, in "Fracture" (H. Liehowitz, ed.), Chap. 2, p. 191. Academic Press, New York, 1968.

<sup>&</sup>lt;sup>18</sup> G. Sih and H. Liebowitz, in "Fracture" (H. Liebowitz, ed.), Chap. 2, p. 67. Academic Press, New York, 1968.

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and Goodier<sup>19</sup> in the series *Fracture*, edited by Liebowitz on the elastic (and plastic) treatment of cracks. Bilby and Eshelby,<sup>16</sup> in a *tour de force*, present cracks entirely in terms of dislocation pileup theory, treating the crack as a distribution of virtual "crack" dislocations in the sense proposed by Friedell.<sup>14</sup> Many reflections of their work will be found in our treatment. Rice<sup>17</sup> has used the Muskhelisvili integral equation in deriving crack stress fields, and because of the similarity of his treatment to ours, his article is especially recommended.

## 7. GENERAL EQUATIONS AND BOUNDARY CONDITIONS<sup>15</sup>

Local static equilibrium at a point in an elastic medium requires that the net force density at the point be equal to zero,

$$f_i = \sigma_{ij,j} = 0, \tag{7.1}$$

where  $\sigma_{ij}$  is the stress tensor, the summation convention over repeated indices is assumed, and the comma represents differentiation. Hooke's law connects the stress with the local derivatives of the displacement (strain), and in an isotropic medium is given by

$$\sigma_{ij} = \lambda u_{i,l} \delta_{ij} + \mu (u_{i,j} + u_{j,l}). \tag{7.2}$$

 $\lambda$  and  $\mu$  are elastic coefficients, and  $u_i(x_1, x_2, x_3)$  is the displacement function.

In any elastic problem, boundary values of  $\sigma_{ij}$  on the external (and internal) surfaces of the body must be specified in order to generate unique solutions. If a surface is free of externally applied forces, the fact that a free surface exists implies that forces,  $F_i$ , cannot be transmitted across it. Thus,

$$F_i = \sigma_{ij} n_j = 0. \tag{7.3}$$

 $n_j$  is the normal vector at the surface pointing from the negative to positive sides of the surface. Equation (7.3) represents the force per: unit area transmitted across the surface from its positive side toward (the material on) its negative side.

In the crack problem (Fig. 16), two general approaches are possible. In the first (Fig. 17a), forces are applied to the external surfaces which give rise to a stress distribution in the body,  $\sigma_{ij}^{(0)}(\mathbf{x})$ . Then a cut is made in the medium which defines the cleavage surface of the crack. Since the cleavage surfaces are free surfaces in the above sense, Eq. (7.3) is satisfied on them. If  $g_{ij,i}(\mathbf{x}, \mathbf{x}')$  is a Green's function for a dipole force at  $\mathbf{x}'$  on the cleavage surfaces (an equal and opposite force is exerted on each of the cleavage surfaces facing one another across the cut), then the total stress in the body in its final stressed and cracked



Fig. 16. Two crack-coordinate configurations for use in this article. In (a), the crack extends indefinitely along the negative  $x_1$  axis. In (b), the crack is finite in length, and again lies along the  $x_1$ axis from  $-a \le x_1 \le +a$ . Dislocations may be present at position  $\zeta_1$  in the complex plane. (c) Construction for Eq. (8.9). An equal and opposite force distribution is exerted on the two surfaces of the cleavage planes in Mode III. These externally applied forces on an element of volume at the upper surface are shown balanced by internally generated at resses, which cancels the total force on the volume element shown.





FIG. 17. Two ways of creating a crack in a medium are illustrated. The stresses may be exerted on the external surfaces as shown in (a), or as a pressure acting within the crack as shown in (b). Under conditions described in the text, the stresses near the crack tips are equivalent.

<sup>19</sup> J. N. Goodier, in "Fracture" (H. Liebowitz, ed.), Chap. 2, p. 2. Academic Press, New York, 1968.

$$\sigma_{ij} = \sigma_{ij}^{(0)} - \int g_{ij,l} \sigma_{ik}^{(0)} n_k \, ds. \tag{7.4}$$

The integral serves the purpose of simply nullifying the forces which were exerted by the initial stresses across the cleavage surface before the cut was made.

In the second approach (Fig. 17b), after the cut is made, forces are exerted on the crack surfaces which force them open, thereby generating stresses in the medium. If  $-\sigma_{lk}^{(0)}n_k$  are these forces, then

$$\sigma_{ij} = -\int g_{ij;t} \sigma_{ik}^{(0)} n_k \, ds \tag{7.5}$$

is the stress in the body. n points from the medium across the surface to the vacuum.

There is thus a basic equivalence between these two approaches, and they will be referred to in the following as Problem 1 and Problem 2. For example, in Mode I, a standard problem is to exert forces on the upper and lower surfaces of the specimen as shown in Fig. 17a, giving rise to a constant stress throughout the body  $\sigma_{ij}^{(0)} = \sigma_{22}^{(0)}$ . In Problem 2, if this same constant force is applied on the surface of the crack, then the only difference between the final stress as given in Eqs. (7.4) and (7.5) is the constant term  $\sigma_{22}^{(0)}$  in Eq. (7.4). Near the crack tips, where most of our concern lies, the stress is highly concentrated, and the constant term can be neglected. Thus, which fracture problem is addressed in any situation is usually a matter of mathematical convenience.

Two-dimensional analysis has a special place in the treatment of fracture problems. The reason is simply that 3D treatments of cracks are usually enormously difficult, and nearly always numerical. Thus, the 3D literature is sparce and recommended for the specialist only. But, as with dislocations, much can be accomplished in 2D, where the crack line is straight (taken along the  $x_3$  axis) and infinite in length. In addition, in 2D, it is required that  $u_{i,3} = 0$  everywhere. Substitution of this requirement into Eq. (7.1) with Eq. (7.2) shows that the solutions break into two separate cases,

$$\nabla^2 u_3 = u_{3,11} + u_{3,22} = 0, \tag{7.6}$$

.

$$(\lambda + \mu)u_{j,\mu} + \mu u_{i,\mu} = 0, \quad i,j = 1,2.$$
 (7.7)

These two cases correspond to the two independent shear and longitudinal polarization solutions for sound waves, and are called antiplane strain, and plane strain, respectively. Equation (7.6) corresponds to screw dislocations and Mode-III cracks, and Eq. (7.7) to edge dislocations and to mode I and II cracks.

There are several approaches to the solution of any boundary-value problem, and, in the case of 2D elasticity, Green's functions, conformal mapping, and a singular integral method generalized from the Hilbert transform have been most effectively used. In any given case, one or another of these techniques can be employed, depending on the case and directness of the relevant mathematics. In cases where the Green's functions can be found easily, that is often the method of choice, but for slit cracks, the singular integral method has been developed by the Russian school associated with Muskhelishvili into an elegant and powerful approach which we shall use, and from which the elastic Green's functions can be derived. On the other hand, conformal mapping can be a powerful tool for application to more general crack shapes such as wedges, which are also important. The mathematics for both these latter approaches will be found in the Appendix. Elasticity is complicated by the tensor character of the variables, and, like electromagnetism, is generally simplified by the introduction of elastic potentials. In spite of the fact that these potentials were discovered in the 19th century, they are not familiar to nonspecialists, and the elastic equations expressed in terms of these potentials are also developed in the Appendix.

In 2D the variables  $u_i$  and  $\sigma_{ij}$  will only be functions of the complex variables  $z = x_1 + ix_2$  and  $\overline{z} = x_1 - ix_2$ , and it is natural to invoke complex function theory. In antiplane strain, where only  $u_3$  is nonzero, this is a particularly straightforward procedure, and it will be discussed first. The reader is reminded, however, since elasticity is a linear theory, that the total solution in mixed cases is a simple superposition of plane and antiplane solutions.

## 8. ANTIPLANE STRAIN. THE MODE-III CRACK

Since the field equation for antiplane strain, Eq. (7.6), is Laplace's Equation, a solution can be given in terms of any analytic complex function  $\eta$  of z, such that

$$u_3 = u_3(x_1, x_2) = (2/\mu) \operatorname{Im}(\eta(z)). \tag{8.1}$$

 $\eta$  will be called the antiplane strain elastic potential and the factor 2 is used to achieve symmetry with certain expressions to be derived in plane strain. The

only nonzero stress components,  $\sigma_{31}$  and  $\sigma_{32}$ , can be written in terms of  $\eta$  by Eq. (7.2) as

$$\sigma(z) = \sigma_{32} + i\sigma_{31} = 2\eta'(z), \qquad (8.2)$$

where the prime denotes differentiation. As shown in the Appendix,  $\sigma$  is not a true vector, because  $\overline{\sigma}/i$  is the quantity which transforms as a vector (see Eq. A.23). In polar coordinates,

$$\sigma_{\sigma_3} = \sigma_{31} \cos \theta + \sigma_{32} \sin \theta = \operatorname{Im}(\sigma e^{i\theta}),$$

$$\sigma_{\sigma_3} = -\sigma_{31} \sin \theta + \sigma_{32} \cos \theta = \operatorname{Re}(\sigma e^{i\theta}).$$
(8.3)

Singular solutions for a dislocation or a line force at the origin are given by

$$\eta = (\mu b/4\pi) \ln z. \tag{8.4}$$

The real part of b represents a dislocation, and the imaginary part gives the strength of a line force. Re (b) is given by the multivaluedness of  $\eta$  at the origin,

$$\mathbf{Re}(b) = \frac{2\Delta\eta}{i\mu} = \frac{2}{i\mu} \oint \eta' \, dz. \tag{8.5}$$

In the same way, the strength of the line force is given by integration of  $\sigma_r$  around the origin.

Suitable elastic potentials for the crack problem are found by satisfying the boundary conditions on the open cleavage surface in Problem 1. If a cleavage plane lies along the negative  $x_1$  axis, with the crack line coinciding with the  $x_3$  axis, as in Fig. 16a, then

$$\sigma_{32}(x_1, 0) = 0, \qquad x_1 < 0. \tag{8.6}$$

A suitable solution is

$$\eta \propto \sqrt{z}, \tag{8.7}$$
$$\eta' = K_{\rm in}/2 \sqrt{2\pi z}.$$

.

In this solution, the cleavage surface is a branch line and  $\sigma \rightarrow 0$  at infinity. The crack tip is a branch point in the function  $\eta$ . This simple result is a clue that crack problems in general will lead to square-root-like functions, with branch lines coincident with the cleavage plane. The discontinuity in the potential function on the cleavage surface corresponds to the discontinuities in both displacement and  $\sigma_{31}$  there. (Note that  $\sigma_{31}$  need not be zero on the open surface along  $-x_1$ .) The constant K is a measure of the strength of the singularity at the crack tip.

In Fig. 16b a more general finite crack is shown lying along the  $x_1$  axis from  $-a \le x_1 \le a$ . Again, a complex potential  $\eta$  is sought having a branch line on the cleavage surface. In Problem II, equal and opposite external forces per unit

area,  $F_{\rm III}(x_1)$ , are exerted on the cleavage plane, as shown in Fig. 16c, thereby generating an internal stress  $\sigma_{32}$ . On an element of volume at the upper surface in Fig. 16c, zero net force requires that  $\sigma_{32}(-n_2^+) + F_{\rm III} = 0$ , with  $n_2^+ = -1$ .  $\sigma_{32}^+ = -F_{\rm III}(x_1)$  on the upper surface. By the same reasoning  $\sigma_{32}^- = -F_{\rm III}(x_1)$  on the lower surface, because equal and opposite forces are exerted on the lower surface. Thus the boundary condition at the cleavage surface is given by

$$[\sigma_{32}]^{+} = [\sigma_{32}]^{-} = -F_{\text{HM}}(x_1), \qquad (8.8)$$

where  $F_{\rm HI}$  is an arbitrary real function of  $x_1$ . In terms of the potential function  $\eta$  Eq. (8.8) is written

$$\{[\eta']^+ + [\eta']^-\} = -F_{\mu\nu}(x_1). \tag{8.9}$$

Note that in Eq. (8.9) the imaginary parts of  $\eta'$  on the opposite sides of the crack surface are of opposite sign, because  $F_{iii}$  is real.

Equation (8.9) and the boundary-value problem it represents conform to the discussion of the Muskhelishvili singular integrals in the Appendix (Subsection 3). Specifically, Eq. (8.9) is of the form specified for h(t) in Eq. (A.40), and the solution for  $\eta'$  according to that equation is

$$\eta'(z) = -\frac{1}{2\pi\sqrt{z^2 - a^2}} \int_{-a}^{a} \frac{F_{\rm in}(t)\sqrt{a^2 - t^2}}{t - z} dt.$$
(8.10)

The polynomial is set to zero in Eq. (A.41) in order for the stress at infinity to be zero. The solution in Eq. (8.10) is singular at  $z = (\pm a, 0)$ . Near z = a, the solution has the form

$$2\eta'(\zeta) = \sigma(\zeta) = \frac{K_{\rm HI}}{\sqrt{2\pi\zeta}} + O\left(\frac{\zeta}{a}\right)^{1/2}; \qquad \zeta = z - a,$$
  
$$K_{\rm HI} = \frac{1}{\sqrt{\pi a}} \int_{-a}^{a} F_{\rm HI}(t) \left(\frac{a+t}{a-t}\right)^{1/2} dt, \qquad (8.11)$$
  
$$K_{\rm HI} = F_{\rm HI} \sqrt{\pi a}; \qquad F_{\rm HI} = \text{const.}$$

This solution corresponds to the "second problem." When a constant stress  $F_{III}$  is added at infinity ("first problem"), the singularities at the crack tips are the same as in Eq. (8.11), and thus the constant  $K_{III}$  is also the same.

The relations in Eq. (8.11) give the central results for the region near a crack tip, showing that a  $1/\sqrt{z}$  stress singularity exists there, with a strength K, called the stress intensity factor. K is linear in the external driving stress, and depends upon the crack geometry, as well as the specimen shape and the way the external stress is applied. This latter point is seen from the second equation of (8.11), where K depends upon the initial stress distribution on the cleavage surface.

The reader will note that Eq. (8.10) has the form of a Green's function solution [Eq. (7.5)], where the Green's function for the finite crack is

$$\eta' = -\int F_{\rm HI}(t)g(t,z)\,dt,$$

$$g(t,z) = \frac{1}{2\pi} \left(\frac{a^2 - t^2}{z^2 - a^2}\right)^{1/2} \frac{1}{t-z}.$$
(8.12)

9. PLANE STRAIN AND PLANE STRESS

The plane-strain equations are given by Eq. (7.7), and in terms of the Goursat potential functions, the field equations (7.7) become

$$\sigma_{11} + \sigma_{22} = 2[\varphi'(z) + \overline{\varphi'(z)}],$$
  

$$\sigma_{22} - \sigma_{11} + 2i\sigma_{12} = 2[\overline{z}\varphi''(z + \psi'(z))],$$
  

$$2\mu u = 2\mu(u_1 + iu_2) = \kappa\varphi(z) - [\overline{z}\overline{\varphi'(z)} + \overline{\psi(z)}].$$
  
(9.1)

These equations are derived in Appendix Subsection 1 [see Eqs. (A.12)-(A.15)].

For cases where the specimen is a plate whose thickness is small compared with all other dimensions in the problem, these same Eqs. (9.1) are also valid, when  $\kappa$  has the appropriate value. This case is called plane stress, and all future equations are valid for both plane strain and plane stress when

$$\kappa = \begin{cases} 3 - 4\nu; \text{ plane strain,} & \sigma_{33} = \nu(\sigma_{11} + \sigma_{22}); \\ (3 - \nu)/(1 + \nu); \text{ plane stress,} & \sigma_{33} = 0. \end{cases}$$
(9.2)

In the fracture problem of Fig. 16, the boundary conditions pertain to  $\sigma_{22}$  and  $\sigma_{21}$ ; so it is convenient to recombine Eq. (9.1) so that these quantities are displayed conveniently:

$$\sigma_{11} + \sigma_{22} = 2[\varphi'(z) + \overline{\varphi'(z)}],$$
  

$$\sigma_{22} - i\sigma_{12} = \varphi' + \overline{\omega'} + (z - \overline{z})\overline{\varphi''}$$
  

$$2\mu u = \kappa \varphi - (z - \overline{z})\overline{\varphi'} - \overline{\omega},$$
  

$$\omega = z\varphi' + \psi.$$
  
(9.3)

In these equations, the new function  $\omega$  has replaced  $\psi$  for convenience in the following analysis, because of the appearance of the term  $(z - \bar{z})$ , which is zero on the  $x_1$  axis.

For a crack lying on the  $x_1$  axis,  $-a < x_1 < a$  (Fig. 16b), in Problem II, the internal stresses on the left-hand side of the second part of Eq. (9.3) are balanced at the crack surface by an externally applied force distribution which we shall call F, and following the reasoning leading up to Eq. (8.10), the

boundary condition on the crack faces where 
$$(z - \overline{z}) = 0$$
 is written

$$-\overline{F} = [\varphi'(t) + \overline{\omega'(t)}]^+,$$
  

$$-\overline{F} = [\varphi'(t) + \overline{\omega'(t)}]^-,$$
  

$$F = F_t + iF_t.$$
(9.4)

As before, + and - superscripts relate to the limiting values of  $\varphi'$  and  $\overline{\omega}'$  on the upper and lower crack surface. In the notation adopted for the externally applied forces,  $F_1$  relates to a force in the  $x_2$  direction producing a Mode-I opening of the crack, and  $F_{11}$  relates to a force in the  $x_1$  direction producing a pure Mode-II crack. The use of the real variable *t* denotes that the variable is taken along the cut,  $-a < x_1 < a$ .

In the form of Eq. (9.4), the Muskhelishvili analysis cannot be used because its right-hand side contains the nonanalytic function  $\overline{\omega}'$ . That is,  $\overline{\omega}$  is not a function of z, but of  $\overline{z}$ . It is, however, possible to rewrite Eq. (9.4) in terms of analytic functions of z, through the function  $\omega^*(z)$  defined by

$$\omega^*(z) = \overline{\omega(\overline{z})}. \tag{9.5}$$

On the real axis, 
$$[\omega^*(t)]^+ = [\overline{\omega(t)}]^-$$
 and Eq. (9.4) becomes

$$[-F]^{+} = [\varphi'(t)]^{+} + [\omega'^{\bullet}(t)]^{-}; [-\bar{F}]^{-} = [\varphi'(t)]^{-} + [\omega'^{\bullet}(t)]^{+}.$$

$$(9.6)$$

Subtraction of these two equations shows that  $[\varphi'(z) - \omega^{\bullet'}(z)]$  is a function with no discontinuity on the crack surface, and hence is analytic everywhere. From Liouville's theorem it is therefore zero, because the constant allowed by Liouville's theorem would not fit the requirement in problem 2 that the stresses are zero at  $\infty$ . Hence,  $\varphi'(z) = \omega^{\bullet'}(z)$ , and the sum of the equations [Eq. (9.6)] has the form

$$-\bar{F} = [\varphi'(t)]^{+} + [\varphi'(t)]^{-}. \qquad (9.7)$$

The analysis of the Appendix Subsection 3 now applies, and the result from Eq. (A.41) is

$$\varphi'(z) = -\frac{1}{2\pi\sqrt{z^2 - a^2}} \int_{-a}^{a} \frac{F\sqrt{a^2 - t^2}}{t - z} dt$$

$$F(t) = F_t(t) + iF_n(t).$$
(9.8)

Investigation of the singularity at z = a leads to

$$\varphi'(\zeta) = \frac{\bar{K}}{2\sqrt{2\pi\zeta}} + O(\sqrt{\zeta/a}),$$

$$K = K_1 + iK_2,$$
(9.9)

$$K = \frac{1}{\sqrt{\pi a}} \int_{-a}^{a} F(t) \left(\frac{a+t}{a-t}\right) dt, \qquad (9.10)$$

in complete analogy to the antiplane-strain case. When  $F_1$  and  $F_2$  are constants,

$$K = F \sqrt{\pi a}.$$
 (9.11)

In this notation, Eqs. (9.9) and (9.10) contain both Mode I and Mode II as their real and imaginary parts, respectively. As noted earlier, Mode-III stresses when they exist are simply added in linear fashion to these equations.

As in the antiplane-strain case, Eq. (9.8) provides an expression for the Green's function for the plane-strain crack, because Eq. (9.8) is in the form of a Green's-function-type integral, with a set of forces,  $\sigma$ , distributed in equal and opposite amounts on the opposing crack surfaces,

$$\varphi'(z) = -\int \bar{F}(t)g(t,z) dt,$$

$$g(t,z) = \frac{1}{2\pi} \left(\frac{a^2 - t^2}{z^2 - a^2}\right)^{1/2} \frac{1}{t-z}.$$
(9.12)

Finally, it is noted that the potential function  $\varphi'(z)$  possesses the same simple form in plane strain as does the  $\eta'$  and stress in antiplane strain. The stresses themselves, however, are quite complicated, and obtained from Eq. (9.3) after a quite tedious manipulation, and this fact demonstrates the great usefulness of the elastic potentials. In the interest of completeness, the stresses are given below:

Equations for Mode I:

Equations for Mode II:

$$\begin{cases} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \\ \sigma_{xy} \\ \end{cases} = \frac{K_{\rm H}}{(2\pi r)^{1/2}} \begin{cases} -[\sin(\theta/2)][2 + \cos(\theta/2)\cos(3\theta/2)] \\ \sin(\theta/2)\cos(\theta/2)\cos(3\theta/2) \\ [\cos(\theta/2)][1 - \sin(\theta/2)\sin(3\theta/2)] \\ (\cos(\theta/2)][1 - \sin(\theta/2)\sin(3\theta/2)] \\ -3\sin(\theta/2)\cos^{2}(\theta/2) \\ (\cos(\theta/2)][1 - 3\sin^{2}(\theta/2)] \\ \cos(\theta/2)[1 - 3\sin^{2}(\theta/2)] \\ \sigma_{xz} = v'(\sigma_{xx} + \sigma_{yy}) = v'(\sigma_{rr} + \sigma_{\theta\theta}), \end{cases}$$
(9.14  
$$\sigma_{xz} = \sigma_{yz} = \sigma_{rz} = \sigma_{\theta z} = 0; \\ u_{z} = -(v''z/E)(\sigma_{xx} + \sigma_{yy}) = -(v''z/E)(\sigma_{rr} + \sigma_{\theta\theta}). \\ u_{x} \\ u_{y} \\ \end{cases} = \frac{K_{\rm H}}{2E} \left(\frac{r}{2\pi}\right)^{1/2} \begin{cases} (1 + v)[(2\kappa + 3)\sin(\theta/2) + \sin(3\theta/2)] \\ -(1 + v)[(2\kappa - 3)\cos(\theta/2) + \cos(3\theta/2)]; \\ (1 + v)[-(2\kappa - 1)\sin(\theta/2) + 3\sin(3\theta/2)] \\ (1 + v)[-(2\kappa + 1)\cos(\theta/2) + 3\cos(3\theta/2)]; \end{cases}$$

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Equations for Mode III:

$$\sigma_{xx} = \sigma_{yy} = \sigma_{rr} = \sigma_{\theta\theta} = \sigma_{xx} = 0, \qquad \sigma_{xy} = \sigma_{r\theta} = 0;$$

$$\sigma_{xx} = \frac{K_{UI}}{(2\pi r)^{1/2}} \begin{cases} -\sin(\theta/2) \\ \cos(\theta/2) \end{cases};$$

$$\sigma_{rx} = \frac{K_{UI}}{(2\pi r)^{1/2}} \begin{cases} \sin(\theta/2) \\ \cos(\theta/2) \end{cases};$$

$$u_{x} = (K_{UI}/2E)(r/2\pi)^{1/2} [2(1 + \nu)\sin(\theta/2)];$$

$$u_{x} = u_{x} = u_{y} = 0 \end{cases}$$
(9.15)

For all modes:

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$$\kappa = (3 - \nu)/(1 + \nu), \quad \nu' = 0, \quad \nu'' = \nu$$
 (for plane stress);  
 $\kappa = (3 - 4\nu), \quad \nu' = \nu, \quad \nu'' = 0$  (for plane strein).

# 10. DISLOCATION STRESS FIELDS

One of the central themes of this article will be the interaction of dislocations with cracks, and in order to study this it will be necessary to develop analytic expressions for the potential function of a dislocation in the presence of a crack. There are a variety of ways for doing this. One is by means

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of the conformal mapping for the known image solutions of dislocations in the presence of an infinite free surface.<sup>20</sup> This is the only method practicable for wedge cracks and other complicated crack shapes. For slit cracks, however, a simpler approach is to use the general Green's-function expressions already developed for slit cracks, Eqs. (8.12) and (9.12).

In both antiplane strain and plane strain, the solution is obtained by breaking  $\eta'$ ,  $\varphi'$ , and  $\omega'$  each into two parts, that given by the dislocation potential in an infinite homogeneous medium, and that required to satisfy the boundary condition at the crack cleavage surface.

a. Antiplane Strain

In antiplane strain, y' is thus given by

$$\eta' = \eta'_0 + \eta'_1,$$
  
 $\eta_0 = \mu b/4\pi (z - \zeta).$ 
(10.1)

The origin is at the tip of the semi-infinite crack shown in Fig. 16a and the screw dislocation is at  $\zeta$ . The solution  $\eta'_0$  produces a nonzero force on the open cleavage surface, and  $\eta'_1$  corresponds to additional forces exerted on the crack plane to ensure that  $\sigma_{ij}n_j = 0$  here. Thus,  $\eta'_1(a)$  is calculated from Eq. (8.10) when that equation is modified to represent the crack configuration of Fig. 16a, i.e., translate the origin to the right-hand side of the crack and take  $a \to \infty$ :

$$\eta'_{1}(z) = \frac{i}{\pi \sqrt{z}} \int_{-\infty}^{0} \frac{\sqrt{t} \operatorname{Re}[\eta'_{0}(t)]}{t-z} dt.$$
 (10.2)

In Eq. (8.10) we have taken  $F_{\rm HI} = -2 \operatorname{Re}[\eta'_0(t)]$  with the substitution for  $\eta'_0$  from Eq. (10.1). Straightforward integration of Eq. (10.2) leads to the total stress

$$2\eta' = \sigma = \frac{\mu}{4\pi\sqrt{z}} \sum_{j} \left( \frac{b_{j}}{\sqrt{z} - \sqrt{\zeta_{j}}} - \frac{b_{j}}{\sqrt{z} - \sqrt{\zeta_{j}}} \right) + \frac{K_{\text{III}}}{\sqrt{2\pi z}} \\ = \frac{\mu}{4\pi} \sum_{j} \left\{ \frac{b_{j}}{z - \zeta_{j}} \left[ \left( \frac{\zeta_{j}}{z} \right)^{1/2} + 1 \right] + \frac{b_{j}}{z - \zeta_{j}} \left[ \left( \frac{\zeta_{j}}{z} \right)^{1/2} - 1 \right] \right\} + \frac{K_{\text{III}}}{\sqrt{2\pi z}}.$$
 (10.3)

In this equation, the total stress is the linear sum of a set of dislocations situated at  $\zeta_j$ , and the crack K field is also added from Eq. (8.7) in order to obtain a general result.

Physically, this expression is interesting because of the appearance of the term in  $\bar{\zeta}_j$ , which corresponds to images of the dislocations at  $\zeta_j$ . Because of

<sup>20</sup> G. Hirth and J. Lothe, "Theory of Dislocations," 2nd Ed. McGraw-Hill, New York, 1982.

the cancelling effect of these images, the dislocation part of the stress field at infinity decays more strongly than the normal 1/z dislocation field. Of course, the overall field is dominated at long range by the  $K_{\rm HI}$  field.

The most important result from Eq. (10.3), however, is that the stress singularity in the tip region is also of the  $1/\sqrt{z}$  variety, but with a different strength than the long-range  $K_{\rm HI}$ . Thus, from the limiting form of  $\sigma$  near the origin, the local stress intensity factor, k, is defined by the relations

$$\sigma_{z \to 0} = k_{\rm HI} / \sqrt{2\pi z},$$

$$k_{\rm HI} = K_{\rm HI} - \frac{\mu}{2} \sum_{j} \left( \frac{b_j}{\sqrt{2\pi \zeta_j}} + \frac{b_j}{\sqrt{2\pi \zeta_j}} \right).$$
(10.4)

The important physical meaning of Eq. (10.4) is that the dislocations shield the crack from the externally applied stress field for positive Burgers vectors. Dislocations with negative Burgers vectors are antishielding dislocations because they enhance the effect of the external field. Note from Eq. (10.4) that  $k_{\rm HI}$ , like  $K_{\rm HI}$ , is always a real quantity.

#### b. Plane Strain

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1. 1

In plane strain, the procedure is exactly the same as the antiplane case, except that two potentials are required,  $\varphi$  and  $\omega$ . As before,

$$\varphi' = \varphi'_0 + \varphi'_1,$$
 (10.5)  
 $\omega' = \omega'_0 + \omega'_1.$ 

 $\varphi'_0$  and  $\omega'_0$  represent the potential functions for "free" edge dislocations. These functions are not exhibited in the traditional dislocation texts, but the reader can verify with Eq. (9.3) that the following expressions reproduce the edge-dislocation stress fields as published, for example, in Hirth and Lothe:<sup>20</sup>

$$\varphi'_{0} = \frac{2A}{z-\zeta},$$

$$\omega'_{0} = \frac{2\bar{A}}{z-\zeta} - \frac{2(\zeta-\bar{\zeta})}{(z-\zeta)^{2}}A,$$

$$A = \frac{\mu b}{2\pi i(\kappa+1)}.$$
(10.6)

These solutions satisfy the Burgers circuit condition and have zero line-force term at the origin. The appearance of the second term in  $\omega'_0$  arises because of the necessary translational symmetry of the stress fields of a dislocation in expressions like Eq. (9.3).

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The terms  $\varphi'_1$  and  $\omega'_1$  are once more chosen to satisfy the boundary condition  $\sigma_{ij}n_j = 0$  on the crack surface in Eq. (9.3). They can again be regarded as due to additional forces exerted on the crack surfaces which accomplish this goal, and which give rise to new stresses calculated from Eq. (9.8). Fortunately, the analysis is simplified, because

$$\varphi_1'(z) = \omega_1^{*}(z). \tag{10.7}$$

The reason is that  $\varphi'_1$  and  $\omega'_1$  are potentials which are derived from ("external") forces exerted on the crack surfaces, and the same reasoning leading up to Eq. (9.7) applies in this case as well. The function  $\overline{F}$  to be used in Eq. (9.8) is given by

$$-F = 2\varphi'_0(t) \tag{10.8}$$

from Eq. (9.3) because  $z = \overline{z}$ . Thus, with the obvious modification of Eq. (9.8) for a semi-infinite crack (translate origin to the right-hand crack tip and let  $a \rightarrow \infty$ ),

$$\varphi_1' = \omega_1'^{\bullet} = \frac{i}{\pi \sqrt{z}} \int_{-\infty}^0 \frac{\sqrt{t} \varphi_0'(t)}{t-z} dt.$$
 (10.9)

The easiest way to evaluate Eq. (10.9) is to integrate in the complex plane,  $\zeta$ , with the expanded contour shown in Fig. 18, in which t is the real axis:

$$\oint_{\infty} = \int_{c} + \oint_{x} + \oint_{\zeta_{0}} + \oint_{\zeta_{0}} = 0.$$
 (10.10)



Fig. 18. Expanded contour of integration of Eq. (10.10) along the negative real axis. The expanded contour surrounds the negative real axis, C, continues at infinity with  $C_{m}$ , and encloses the poles at z,  $\zeta_{0}$ , and  $\overline{\zeta}_{0}$ .

The final result for the total  $\varphi'$  corresponding to a collection of dislocations in the presence of a crack is

$$\varphi' = \varphi'_{0} + \varphi'_{1}$$

$$= \sum_{j} A_{j} \left\{ \frac{1}{z - \zeta_{j}} \left[ \left( \frac{\zeta_{j}}{z} \right)^{1/2} + 1 \right] + \frac{1}{z - \overline{\zeta_{j}}} \left[ \left( \frac{\overline{\zeta_{j}}}{z} \right)^{1/2} - 1 \right] \right\}$$

$$+ \sum_{j} \frac{\overline{A}(\zeta_{j} - \overline{\zeta_{j}})^{2}}{2(z - \overline{\zeta_{j}})^{2}} \left[ \left( \frac{\overline{\zeta_{j}}}{z} \right)^{1/2} + \left( \frac{z}{\overline{\zeta_{j}}} \right)^{1/2} - 2 \right]$$

$$+ \frac{\overline{K}}{2\sqrt{2\pi z}}; \quad K = K_{1} + iK_{11}; A_{j} = \mu b_{j}/2\pi i(\kappa + 1). \quad (10.11)$$

For ω',

$$\omega' = \sum_{j} \bar{A}_{j} \left\{ \frac{1}{z - \zeta_{j}} \left[ \left( \frac{\zeta_{j}}{z} \right)^{1/2} + 1 \right] + \frac{1}{z - \zeta_{j}} \left[ \left( \frac{\bar{\zeta}_{j}}{z} \right)^{1/2} - 1 \right] \right\} - \sum_{j} \frac{A_{j} (\zeta - \bar{\zeta}_{j})}{2(z - \zeta_{j})^{2}} \left[ \left( \frac{\zeta_{j}}{z} \right)^{1/2} + \left( \frac{z}{\zeta_{j}} \right)^{1/2} + 2 \right] + \frac{K}{2\sqrt{2\pi z}}.$$
 (10.12)

As in the antiplane-strain case, the relevant expression for the crack part of the potentials, in Eq. (9.9) have been added to Eqs. (10.11) and (10.12), and the additive property of stresses has been used to write an expression for a collection of dislocations of Burgers vectors  $b_j$  at positions  $\zeta_j$ . These equations for the potentials  $\varphi$  and  $\omega$  exhibit some similarities to the antiplane-strain case, Eq. (10.3), but contain extra terms. As in the antiplane-strain case, the dominant term at infinity in these equations is the K term. The far-field stresses of the dislocations are also again degraded by the image terms in the crack surface, although these image terms are considerably more complicated than in the earlier case.

The limiting functional form of Eqs. (10.11) and (10.12) at infinity and at the origin again provides the basis for the physical picture in which the dislocations shield or antishield the crack. The relation between local and applied stress intensity factors is then given by

$$\varphi_{s \to 0} = \bar{k}/2\sqrt{2\pi z}$$

$$\bar{k} = \bar{K} - \frac{\mu}{2i(1-\nu)} \sum_{j} \left( \frac{b_{j}}{\sqrt{2\pi\zeta_{j}}} + \frac{b_{j}}{\sqrt{2\pi\zeta_{j}}} + \frac{\pi \bar{b}_{j}(\zeta_{j} - \bar{\zeta}_{j})}{(2\pi\zeta_{j})^{3/2}} \right). \quad (10.13)$$

The reader is reminded of the complex number character of k, K, and  $b_j$ ;  $k = k_1 + ik_{11}$ ;  $b = b_1 + ib_2$ , etc. [As noted earlier, these equations are valid for plane stress when the substitution  $v \rightarrow v/(1 + v)$  is made.]





A somewhat different treatment from that given here for dislocation-crack stresses is given by Hirth and Wagoner,<sup>21</sup> and an elegant method for deriving the image stress of dislocations in the presence of cracks [contained in Eqs. (10.11), (10.12), and (10.3)] has been derived by Rice and Thomson.<sup>22</sup> The method here is quite similar to, and was suggested by, a development in unpublished lecture notes of J. R. Rice.

### 11. WEDGE CRACKS

Although in most crack problems, the slit-crack analysis is adequate because dislocation processes at the crack tip modify its shape, dislocation interactions with other shapes are important. In particular, the wedge configuration is the result of continued dislocation emission (see Fig. 11), and will be dealt with here. The analysis will follow that of Chang *et al.*,<sup>23</sup> but Sinclair<sup>24</sup> has also discussed the dislocation-wedge configuration, numerically. As mentioned earlier, the only analytic method suitable for this case is conformal mapping as presented in the Appendix (Subsection 2). The geometry is shown in Fig. 19.

In antiplane strain, the relevant equations are Eqs. (A.27) and (A.28). The boundary condition, of course, is that  $\sigma_{ij}n_j = 0$ , which transforms into the  $\xi$ 

plane as

$$Im[\sigma_{\tau}(re^{\pm i\pi/2})] = 0. \tag{11.1}$$

The transformation law is

$$c = \xi^{\mu}, \quad 1 (11.2)$$

where p is geometrically related to the wedge geometry as shown in Fig. 19, and points on the wedge are transformed onto the imaginary axis of the plane. Equation (A.28) becomes

$$\sigma_{\rm T}(\xi) = \frac{2}{p(\bar{\xi}\xi)^{(p-1)/2}} \frac{d\eta(\xi)}{d\xi},$$

$$e^{i\alpha} = \left(\frac{z'(\xi)}{\bar{z}'(\xi)}\right)^{1/2} = \left(\frac{\xi^{p-1}}{\bar{\xi}^{p-1}}\right)^{1/2}.$$
(11.3)

 $\alpha$ , as explained in the Appendix, is the local rotation at a point.

Since  $\xi \bar{\xi}$  is a real quantity everywhere, the boundary condition on the  $x_2$  axis in the plane is then

$$\operatorname{Im}[\eta'(\xi)]_{\operatorname{Im}\operatorname{axis}} = 0. \tag{11.4}$$

A second boundary condition, of course, is that the solution represent a dislocation at  $z = \zeta$  in the z plane; that is u(z) must be double valued at  $\zeta$  with strength given by the Burgers vector

$$\Delta u(z=\zeta)=b. \tag{11.5}$$

These two boundary conditions, of course, are reminiscent of the similar problem of the image solution for a dislocation in an infinite free surface, and indeed the function,

$$\eta(\xi) = \frac{A}{2} \ln \left( \frac{\xi - \zeta^{1/p}}{\xi - \bar{\zeta}^{1/p}} \right)$$
(11.6)

satisfies Eq. (11.4). The constant  $\zeta^{1/p}$  is chosen so that  $\eta(z)$  is singular at  $z = \zeta$ . In the z plane, Eq. (11.5) is satisfied if A takes the form

$$\eta(z) = \frac{\mu b}{4\pi} \ln\left(\frac{z^{1/p} - \zeta^{1/p}}{z^{1/p} - \zeta^{1/p}}\right), \qquad (11.7)$$
  
$$\sigma(z) = 2\eta'(z).$$

This function is the same as the crack solution [Eq. (10.3)] when p = 2.

The dislocation interaction with a wedge is only complete when a term corresponding to a K term in Eq. (10.3) is added. When the wedge (assumed semi-infinite in extent) is present without a dislocation, Eq. (11.4) is still valid,

<sup>21</sup> J. Hirth and R. Wagoner, Int. J. Solids Struct. 12, 117 (1976).

<sup>22</sup> J. Rice and R. Thomson, Philos. Mag. 29, 73 (1974).

<sup>&</sup>lt;sup>23</sup> S. Chang, S. Ohr, and R. Thomson, to be published (1986).

<sup>24</sup> J. Sinclair, Nucl. Metall. 20, 388 (1976).

and the simplest function satisfying Eq. (11.4) is

$$\eta' = \frac{p}{2} \Lambda_{uu}; \qquad \eta = \frac{p}{2} \Lambda_{uu} \xi, \qquad \xi \text{ plane};$$
  
$$\eta' = \frac{\Lambda_{uu}}{2z^{1-1/p}}; \qquad \eta = \frac{p}{2} \Lambda_{uu} z^{1/p}, \qquad z \text{ plane}.$$
 (11.8)

This solution has the same meaning and limitations as the infinite crack solution [Eq. (8.8)] has. That is,  $\Lambda_{iii}$ , as a measure of the strength of the wedgetip singularity, must be specified by other considerations, such as those discussed in Part III,3. Note that for p = 2,  $\Lambda_{\rm HI} = K_{\rm HI} / \sqrt{2\pi}$ .

In antiplane strain, the total potential function for dislocations and "loaded" wedge is given by the linear superpositions

$$\eta(z) = \sum_{j} \frac{b_{j}}{4\pi} \ln\left(\frac{z^{1/p} - \zeta_{j}^{1/p}}{z^{1/p} + \zeta_{j}^{1/p}}\right) + \frac{p}{2} \Lambda_{\rm su} z^{1/p}$$
(11.9)

## 12. ANISOTROPIC ELASTICITY

General methods have been developed for anisotropic elastic problems and have been applied primarily to dislocations. An excellent recent review of these techniques is provided by Bacon et al.<sup>25</sup> For two-dimensional problems, this theory is based on the methods originated by Eshelby et al.,<sup>26</sup> which are briefly summarized below. In the general tensor notation for Hooke's law,

$$\sigma_{ij} = c_{ijkl} u_{k,l}. \tag{12.1}$$

The equations of equilibrium are

$$\sigma_{ij,j} = 0 = \sigma_{ijkj} u_{k,ij}. \qquad (12.2)$$

If all derivatives with respect to  $x_3$  are zero, then a solution of the equations is

$$u_k = A_k f(p_1 x_1 + p_2 x_2). \tag{12.3}$$

Substitution of Eq. (12.3) into (12.2) yields a set of homogeneous algebraic equations in the coefficients,

$$c_{ijkl}p_ip_lA_k = 0. \tag{12.1}$$

In this notation,  $p_3 = 0$ , and because of the arbitrary form of the function f, it is permissible to set  $p_1 = 1$ . With this convention, the determinant for the coefficients in Eq. (12.4) when set to zero yields a sixth-order polynomial in  $p_2$ ,

<sup>25</sup> D. J. Bacon, D. M. Barnett, and R. D. Scattergood, Prog. Mater. Sci. 23, 51 (1980).

10 J. Eshetby, W. Read, and W. Shockley, Acta Metall. 1, 251 (1953).

which will yield complex roots. Because the  $c_{ijkl}$  in Eq. (12.2) are all real, the roots of the determinantal equation appear in complex-conjugate pairs. Thus, there are three independent values of  $p_2$ , for which it has been customary to introduce a notation with Greek indices,  $p_{2a}$ , in which the summation convention does not apply to repeated Greek indices. With these conventions. the general solution has the form

$$u_k = \sum_{a=1}^{n} A_k f_k(x_1 + p_{2a} x_i).$$
(12.5)

Since  $u_k$  is real, the two f's corresponding to complex conjugate p's are also paired, so that the final solution is

$$u_{k} = \sum_{a=1}^{3} \operatorname{Re} A_{k} f_{a}(x_{1} + p_{2a}x_{2}). \qquad (12.6)$$

Thus there are three arbitrary solutions,  $f_a$ , of a complex variable  $z_a =$  $[x_1 + \operatorname{Re}(p_{2e})x_2] + i \operatorname{Im}(p_{2e})x_2$ , and the usual complex function theory can be employed.

In particular, the stresses are given by the relations

$$\sigma_{i1} = 2 \operatorname{Re} \left( -\sum_{a=1}^{3} p_a L_{ia} f'_a(z_a) \right),$$
  

$$\sigma_{i2} = 2 \operatorname{Re} \left( \sum_{a=1}^{3} L_{ia} f'_a(z_a) \right).$$
(12.7)

f' denotes differentiation with respect to  $z_n = x_1 + p_2 x_2$ . This theory has been applied to the crack problem by a number of authors, with results as reviewed by Bacon et al.25

A general warning must be made in applying this formalism in certain cases. In the isotropic case, the solutions become highly degenerate, and isotropic results are not always the limit of the corresponding anisotropic expressions. For example, in the isotropic case, antiplane strain separates from plane strain. and in plane strain, the solution [Eq. (12.3)] is not the most general solution of Eq. (12.2). Additional functions are required. Thus, in plane-strain isotropic problems it is best to revert to the Airy stress-function analysis or its complexvariable variant as done in this section.

## IV. The Elastic Forces on Cracks and Dislocations

### 13. INTRODUCTION

Since the problem of fracture entails the traversal of a crack and its associated dislocated deformation zones through a solid, the problem of the equilibrium configuration and dynamics of the assemblage requires an analysis couched in terms of the various forces on and between the constituent defects. Historically, the elastic force on a dislocation segment was worked out many years ago by Peach and Koehler,<sup>27</sup>

$$d\mathbf{f} = (\mathbf{\sigma} \cdot \mathbf{b}) \times d\mathbf{l} \tag{13.1}$$

in terms of the external stress field  $\sigma$ , the Burgers vector b, and the line segment dl. A fundamental result of Peach and Kochler's analysis is that the self-stress of the dislocation does not exert a force on itself. Likewise, for the elastic sharp crack, Irwin<sup>28</sup> derived a similarly classic result for the force per unit length on a Mode-I crack in two-dimensional isotropic elasticity, in terms of the stress intensity K, Poisson ratio v, and Young's modulus E,

$$f = K_1^2 (1 - v^2) / E.$$
 (13.2)

This force is traditionally called the energy release rate in the mechanics literature, and is known by the letter G. However, here we adopt a more comfortable physical notation.

When cracks and dislocations are combined together, as in nearly all fracture events, one could proceed by simply combining these two results in an ad hoc manner to find the individual forces on cracks and/or dislocations, because from Part III, the stress fields and local stress intensity factors are known. However, there is a more powerful, general, and elegant approach which follows from the basic theorem of Eshelby<sup>29</sup> on the force exerted on an elastic singularity, expressed in terms of the energy momentum tensor for the elastic field. This second approach has the added advantage that it can be written in terms of the complex potentials, which are much simpler to work with than the full stress tensors as in Eq. (13.1). With it, we shall also make direct contact with the J integral of Rice, 30-32 which is the standard continuum-mechanics approach to cracks in a deformation field. Clearly, then, we shall prefer this latter path, and will display the Peach-Koehler and Irwin results as special cases. The point of view and results of this section largely stem from two papers involving the author. 33,34

<sup>27</sup> M. O. Peach and J. S. Koehler, Phys. Rev. 80, 436 (1950).

28 G. R. Irwin, J. Appl. Mech. 24, 361 (1957).

29 J. D. Eshelby, Solid State Phys. 3, 79 (1956).

30 J. Rice, J. Appl. Mech. 35, 13 (1968).

31 J. R. Rice, in "Fracture" (H. Liebowitz, ed.), Chap. 2, p. 191. Academic Press, New York, 1968.

<sup>37</sup> J. Rice, Mech. Fract. ASME Winter Annu. Meet., 1976; AMD 19, 33 (1976).

<sup>33</sup> R. Thomson and J. Sinclair, Acta Metall. 30, 1325 (1982).

34 1. H. Lin and R. Thomson, Acta Metall. 34, 187 (1986).

# 14. THE FORCE ON AN ELASTIC SINGULARITY: ESHELBY'S THEOREM

To derive this theorem, following Eshelby,<sup>29</sup> we suppose the finite elastic body possesses a set of stress singularities, as shown in Fig. 20, and that the external surface of the body is subjected to a specified set of external forces. A strain-energy density function is assumed to exist, and since, except at the singularities, the medium is elastic, this function is given by

$$W = \frac{1}{2}\sigma_{ij}u_{i,j}.\tag{14.1}$$

In this and the following equations through (14.8), the full three-dimensional elastic notation will be used. If all the singularities move a constant distance  $\delta x$ from their initial positions x, to  $x_{\mu} + \delta x$ , the energy change is calculated in three stages:

In Stage I, the energy change,  $\delta U^{(1)}$ , arises from integrating the strainenergy density function over the solid. In this stage, when the sources translate, the stresses and displacements constituting the elastic solution are assumed to move rigidly with them in space. Thus, after the displacements occur, the new value of the strain-energy function is

$$W^{(1)}(x) = W(x) - \frac{\partial W}{\partial x_k} \delta x_k. \qquad (14.2)$$



FIG. 20. Figure for deriving Eshelby's theorem. A body is contained within an external surface S, and is subject to external stresses. Strain singularities exist at s1, s2, s3,..., which are translated by  $\delta x$  to new positions.  $S_i$  is an inner surface enclosing singularities  $s_1$  and  $s_2$ .

$$-\frac{\partial W}{\partial x_k}\delta x_k. \tag{14.2}$$

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The total energy change integrated over the body is thus by Gauss's theorem

$$\delta U^{(1)} = -\int \frac{\partial W}{\partial x_k} \delta x_k \, dV = -\int W \, dS_k \, \delta x_k. \tag{14.3}$$

In the second stage, the boundary condition on the surface of the body when the sources translate is considered. In Stage 1, just above, when the elastic solutions translate rigidly with the sources, the stresses at the boundary translate in the same way. However, although the stress originally on the boundary satisfied the required boundary condition,

$$\sigma_{ij}n_j = F_i, \tag{14.4}$$

on the boundary, where n is the normal to the boundary, after the rigid translation of the elastic solution, the new stresses and displacements on the boundary no longer satisfy Eq. (14.4). In Stage 2, an additional surface stress is generated, such that when it is added to the translated stress, the total stress satisfies the required condition [Eq. (14.4)], on the surface. The added stress,  $\Delta \sigma_{ij}$ , generates a new set of displacements at the surface after the translation has taken place. Thus, if  $u^{(0)}$  is the initial displacement before the sources are displaced, the changes generated in displacements during Stage 2 are

$$\Delta u_i = u_i^{\text{final}} - \left( u_i^{(0)} - \frac{\partial u_i^{(0)}}{\partial x_j} \delta x_j \right). \tag{14.5}$$

The work done on the body by the total stress acting over  $(\Delta w_i)$  is then, to first order ( $\sigma + \Delta \sigma \sim \sigma$ ),

$$\begin{aligned} \delta U^{(2)} &= \int \sigma_{ij}^{(0)} \Delta u_j \, dS_j \\ &= \int \sigma_{ij}^{(0)} \left( u_i^{final} - u_j^{(0)} + \frac{\partial u_i}{\partial x_k} \delta x_k \right) dS_j. \end{aligned}$$
(14.6)

The third contribution is the energy change in the external loading machinery caused by the total change in displacement at the surface,  $u^{(ins)} - u^{(0)}$ . This is the total change in displacement from that before the source translates to that after the end of Stage 2, when the boundary conditions are satisfied

$$\delta U^{(3)} = -\int \sigma_{ij}^{(0)} \left( u_i^{(\text{inal}} - u_i^{(0)} \right) dS_j.$$
 (14.7)

Addition of Eqs. (14.3), (14.6), and (14.7) gives the final result

$$f_{k} = -\frac{\partial U}{\partial x_{k}} = \int (W \delta_{ik} - \sigma_{ij} u_{i,k}) dS_{j}. \qquad (14.8)$$

 $f_k$  is the force on the singularity in the Lagrangian sense because it represents the negative of an energy derivative.

A subtlety arises when applying Eq. (14.8) to a crack. The slit comprising the cleavage plane of the crack is, of course, a part of the external surface of the body. However, since on the free surface of the slit, Eq. (14.4), is satisfied, the second term in Eq. (14.8) is zero. Also, by symmetry, W on the lower surface is equal to W on the upper. Because of the change in sign of  $dS_i$  when comparing the upper to the lower surface, the contribution of the first term is thus zero also. Hence, in making a contour around a crack, the contour may end on the crack cleavage surface.

The integration in Eq. (14.8) is over the actual external surface of the body, and may enclose a number of singularities. The force in this case represents the total force on the entire set of singularities. If instead, the force on a single singularity, or subset of the original group, is desired, the following strategem can be adopted. An inner boundary,  $S_i$ , is drawn surrounding the singularities in question (Fig. 20), and the remainder of the body then serves as an "external driving system" on the inner surface. In carrying out Stage 2 of the argument, however, a subtle point must be observed. The boundary conditions are established on the real surfaces of the body, and the  $\Delta u_i$  as calculated in Eq. (14.5) are the  $\Delta u_i$  on the inner integration path  $S_i$  which are induced by satisfying the boundary conditions on the external surface S. The rest of the argument then follows as before. In this case, of course, the force on the singularities within S<sub>i</sub> is not only a function of the external driving stresses, but also of the remaining singularities outside  $S_i$ .

An important property of the integral in Eq. (14.8) is that, within certain limits, it is independent of the shape of the surface. Consider two surfaces enclosing a collection of singularities, such that the volume between the two surfaces contains no additional singularities. Then the difference in the integration over the two surfaces is

$$f_k^{I} - f_k^{II} = \oint (W \delta_{ik} - \sigma_{ij} u_{i,k}) dS_j, \qquad (14.9)$$

where the integral now encloses the volume between the two surfaces. Using Gauss's law for the enclosed volume, the equation of equilibrium,  $\sigma_{ij,j} = 0$ , and remembering that within V there are no additional singularities, then

$$f_{k}^{i} - f_{k}^{ii} = \int_{V} (W_{,k} - \sigma_{ij} u_{i,kj}) dV. \qquad (14.10)$$

The general definition of the strain-energy density is

$$W = \int \sigma_{ij} d\epsilon_{ij}; \quad \epsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}). \quad (14.11)$$

By the chain rule of differentiation, and provided that  $\sigma_{ij}$  is only a function of the strain function  $\varepsilon_{ij}$ , which does not depend upon position (i.e., the medium is elastically homogeneous), then

$$W_{,k} = \epsilon_{ij,k} \frac{d}{d\epsilon_{ij}} \int \sigma_{nl} d\epsilon_{nl} = \sigma_{ij} u_{j,kl}, \qquad (14.12)$$

and the integral in Eq. (14.11) is zero. Hence Eq. (14.8) depends only on the number, type, and configuration of singularities enclosed in the contour for a homogeneous medium, and does not depend upon the shape of the contour. In more physical terms, if  $f_k$  in Eq. (14.8) is the Langrangian force on the singularities, it cannot depend upon the shape of the contour on which the elastic fields are evaluated.

This corollary is very evocative of the Cauchy residue theory in two dimensions, and indeed it has been shown<sup>33</sup> that for general anisotropic media Eq. (14.8) can be written in two dimensions as

$$f_{i} = -4\pi \ln\left(\sum_{e=1}^{3} (\pm p_{ie} L_{kl} A_{ke}) \sum_{\text{Res}} \operatorname{Res}[f'_{e}(z_{e})]^{2}\right).$$
(14.13)

This equation is written in the notation of Stroh<sup>35,36</sup> explained in Part III,12, and  $\sum_{Res}$  is a sum over the enclosed residues. The  $\pm$  sign is the sign of Im( $p_{a}$ ). The Peach-Koehler and Irwin relations are also examples of the same proposition that forces on defects depend only on functions evaluated at the singularities.

# 15. ANTIPLANE STRAIN, MODE-III AND SCREW DISLOCATIONS

In isotropic elasticity, the general equation (14.13) degenerates into noninteracting antiplane- and plane-strain parts. The antiplane-strain part then corresponds  $^{35,36}$  to

$$p_{3} = i,$$

$$L_{k3} = \frac{1}{2}\delta_{k3},$$

$$A_{k3} = -\delta_{k3}/2\mu,$$

$$(15.1)$$

$$T'_{3}(z) = \sigma(z),$$

<sup>35</sup> A. N. Stroh, Philos, Mag. 3, 625 (1958).
 <sup>36</sup> A. N. Stroh, J. Math. Phys. 41, 77 (1972).

where  $\sigma(z)$  is the complex stress defined in Eq. (8.2). Then Eq. (14.13) becomes

$$\bar{f} = \frac{\pi}{\mu} \sum_{\text{Res}} \text{Res}(\sigma^2),$$

$$f = f_1 + if_2.$$
(15.2)

Alternatively, one can derive Eq. (15.2) directly from Eq. (14.8) using the complex function notation of Part III, by substitution for  $\sigma_{ij}$  and  $u_i$  in antiplane strain, and using the Cauchy residue theorem. Note the complex vector notation introduced for the force f.

The simple Irwin and Peach-Koehler relations are recovered from Mode-III cracks and screw dislocation by taking a contour surrounding only one defect in each case. For a Mode-III crack at the origin, from Eq. (8.11),  $\sigma = K_{\rm HI}/\sqrt{2\pi z}$ , and

$$\tilde{f}_{c} = K_{\rm in}^2/2\mu.$$
 (15.3)

This equation is the Mode-III form of the Irwin relation. Note that the force is real, so the crack opens only in the x, direction.

For a dislocation, the self-stress is of the form 1/z, which contributes no residue. Thus the self-force is zero. If an analytic external stress  $\sigma_0$  is added to the dislocation stress, so that

$$\sigma = \sigma_0(z) + \mu b/2\pi z, \qquad (15.4)$$

then the force on the dislocation becomes

$$\bar{f} = b\sigma_0, \tag{15.5}$$

which is again the Peach-Koehler result.

More substantive results are obtained when the crack coexists with one or more dislocations. For this purpose the stress field of Eq. (10.3) is required. Using this expression in Eq. (15.2), the force on the crack is

$$\bar{f}_{e} = k_{\rm HI}^2 / 2\mu,$$

$$k_{\rm HI} = K_{\rm HI} - \frac{\mu}{2} \sum_{J} \left( \frac{b_J}{\sqrt{2\pi \zeta_J}} + \frac{b_I}{\sqrt{2\pi \zeta_J}} \right).$$
(15.6)

Thus the force is the expected Irwin relation, but using the local k field of the crack, as defined in Eq. (10.4). Note again that the force is always real, that is,  $\overline{f}$  is an extension force along the x, direction. In antiplane strain, there is no force tending to carry the crack away from its initial cleavage plane.

The force on a dislocation at  $\zeta$  with Burgers vector b in the presence of the crack and other dislocations at  $\zeta_j$  with Burgers vector  $b_j$  as shown in Fig. 21 is

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FIG. 21. Crack-dislocation configuration. In this section, the crack is assumed to lie along the negative real axis. Dislocations are located at points  $\zeta_j$ . When a reference dislocation is needed, as for example when a force is calculated on it, it is referred to without subscript. Subscripts are given to all other dislocations.

evaluated in terms of the residue at  $\zeta$ , and is given by

$$\tilde{f}_{d} = \frac{K_{11}b}{\sqrt{2\pi\zeta}} - \frac{\mu b^{2}}{4\pi} \left[ \frac{1}{2\zeta} + \frac{1}{\zeta - \zeta} - \left(\frac{\bar{\zeta}}{\zeta}\right)^{1/2} \frac{1}{\zeta - \zeta} \right] + \sum_{j} \frac{\mu bb_{j}}{4\pi} \left[ \frac{1}{\zeta - \zeta_{j}} - \frac{1}{\zeta - \bar{\zeta}_{j}} + \left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} \frac{1}{\zeta - \zeta_{j}} + \left(\frac{\bar{\zeta}_{j}}{\zeta}\right)^{1/2} \frac{1}{\zeta - \bar{\zeta}_{j}} \right]$$
(15.7)

The prime on the summation is to remind one that the reference dislocation at  $\zeta$  is not included.

Three types of terms are contained in Eq. (15.7). The first is the K field, or direct crack interaction and depends on the distance from the crack as  $1/\sqrt{\xi}$ . The second is a self-image force on the dislocation in the open surface of the crack, because it depends only on b and varies with distance from the tip as  $1/\zeta$ . Further, the self-image force in the radial direction from the crack is simply

$$(f_r^a)_{image} = -\mu b^2 / 4\pi |\zeta|, \qquad (15.8)$$

which is exactly the same as if, at the crack line, an infinite open surface were erected perpendicular to the radius to the dislocation. This is a result first obtained by Rice and Thomson.<sup>37</sup> The third group of terms is the contribution to the force from the dislocation-dislocation interactions. They have the expected  $1/(\zeta - \zeta_j)$  terms, but are modified by the factors  $\sqrt{\zeta/\zeta_j}$ , because, if the reference dislocation is near the crack tip, even if  $K_{111} = 0$ , it will sense a stress concentration there contributed by the stresses of the dislocations at  $\zeta_j$ . These are, of course, the K-field contributions due to the dislocations which lead to the local k concept in Eq. (15.6). In addition to the direct dislocationdislocation terms, there are also contributions from dislocations at the image points,  $\overline{\zeta}_j$ , and caused by the open surface on the cleavage plane. Note particularly that the sign of the force is linear in b in the first term, bilinear in the third term, and is quadratic in the second. That is, the force is repulsive or attractive, depending on b or  $b_i$  in the first or third terms, but always attractive for the self-image term.

An interesting variation of Eq. (15.7) can be written in terms of the local  $k_{\rm HI}$ , namely

$$\bar{f}_{d} = \frac{k_{\rm HI}b}{\sqrt{2\pi\zeta}} + \frac{\mu b^{2}}{4\pi} \left[ \frac{1}{2\zeta} - \frac{1}{\zeta - \zeta} + \left(\frac{\zeta}{\zeta}\right)^{1/2} \frac{1}{\zeta - \zeta} \right] + \sum' \frac{\mu bb_{j}}{4\pi} \left[ \frac{1}{\zeta - \zeta_{j}} - \frac{1}{\zeta - \zeta_{j}} + \left(\frac{\zeta}{\zeta_{j}}\right)^{1/2} \frac{1}{\zeta - \zeta_{j}} + \left(\frac{\zeta}{\zeta_{j}}\right)^{1/2} \frac{1}{\zeta - \zeta_{j}} \right]. \quad (15.9)$$

Thus, Eq. (15.7) is a form which best expresses the force when the dislocation is near the outer edge of the dislocation distribution, while Eq. (15.9) is a better approximation when near the inner edge.

When the contour is taken around all dislocations and the crack, then the result is simply

$$Rc(\bar{f}_{iot}) = K_{ill}^2 / 2\mu.$$
(15.10)

Thus the elastic force on the entire collection of crack plus dislocations is simply that for a crack characterized by the far field K. When the distribution is symmetric about the real axis, then  $Im(f_{red}) = 0$ .

A simple relation can be written when all the dislocations are lined up on the  $x_1$  axis in a one-dimensional distribution. Then Eq. (15.7) becomes

$$\bar{f}_{d} = \frac{K_{\rm III}}{\sqrt{2\pi x}} - \frac{\mu b^2}{4\pi x} + \sum_{j}' \frac{\mu b b_j}{2\pi (x - x'_j)} \left(\frac{x'_j}{x}\right)^{1/2},$$
(15.11)

$$K_{\rm III} = k_{\rm III} + \sum_{I} \frac{\mu o_I}{\sqrt{2\pi x_I}}.$$

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The simplicity of this result lends itself to use in pileup problems in later sections.

# 16. PLANE STRAIN: EDGE DISLOCATIONS AND MODE-I AND MODE-II CRACKS

The Mode-I and Mode-II case is not a straightforward limit of the anisotropic results as in antiplane strain, because the isotropic solutions of the field equations are not of the form of Eq. (12.13). It is then necessary to revert to the potential functions developed in Parts III,9 and 11. With the use of the strain-energy function in its plane-strain form,

$$W = \frac{1}{2}\sigma_{ij}u_{i,j} = \frac{1}{2}[\sigma_{11}u_{1,1} + \sigma_{12}(u_{2,1} + u_{1,2}) + \sigma_{22}u_{2,2}], \quad (16.1)$$

direct substitution of the stresses and displacements, Eq. (9.3), into (14.8) can

<sup>&</sup>lt;sup>37</sup> J. Rice and R. Thomson, Philos. Mag. 29, 73 (1974).

be shown to yield 34

$$=\frac{2\pi(1-\nu)}{\mu}\sum_{\text{Res}}\left[2\operatorname{Res}(\varphi'\omega'-\varphi^2-z\varphi'\varphi'')+\operatorname{Res}(\varphi^2)\right].$$
 (16)2)

In terms of the  $\varphi$  and  $\psi$ ,  $\overline{f}$  has the simpler form

$$\tilde{f} = \frac{2\pi(1-\nu)}{\mu} \sum_{\text{Res}} [2 \operatorname{Res}(\varphi'\psi') + \overline{\operatorname{Res}(\varphi'^2)}]. \qquad (16.\beta)$$

Similar equations have also been derived by Budiansky and Rice,  $^{30}$  and by Chang.  $^{39}$ 

For the crack alone, the force corresponds to the residue at the origin, and carrying out a limit analysis of Eqs. (12.6) and (12.7) at the origin, the force on the crack is

$$\bar{f}_{c} = \frac{1 - v}{2\mu} \left( k\bar{k} + \frac{k^{2} - \bar{k}^{2}}{2} \right),$$

$$k = k_{1} + ik_{1}v.$$
(16.4)

The k here is the local k at the crack tip. In terms of components,

$$(f_{\rm e})_{\rm I} = \frac{1-\nu}{2\mu} (k_{\rm I}^2 + k_{\rm I}^2) = \frac{1-\nu^2}{E} (k_{\rm I}^2 + k_{\rm I}^2), \qquad (16.5)$$

$$(f_c)_2 = -\left(\frac{1-\nu}{\mu}\right) k_1 k_0. \tag{16.6}$$

E is Young's modulus. Equation (16.5) is the Irwin relation for Modes I and II.

Unlike Mode III, there is in Eq. (16.6) a component of the force along the imaginary axis, the meaning of which is somewhat obscure. Strictly speaking, Eq. (16.6) is the force of translating the crack rigidly in the  $X_2$  direction, which is not a normal physical motion for the crack. However, cracks dolbranch away from their original cleavage planes, as shown in Fig. 22. One might suppose that Eq. (16.6) would form a reasonable estimate of this branching force, since the force on the crack is the same as the force on the virtual or "crack" dislocations which are equivalent to the crack, and these dislocations are highly concentrated at the tip. But a more careful analysis of the branching force shows that such is not the case, and that the branching force is actually composed of a linear combination of the terms  $k_1^2$ ,  $k_{11}^2$ , and  $k_1k_{11}$  in an approximate treatment carried out by Cottrell and Rice.<sup>40</sup> The reader is

38 B. Budiansky and J. Rice, J. Appl. Mech. 40, 201 (1973).

<sup>39</sup> S. J. Chang, Int. J. Fract. 16, R79 (1980).

40 B. Cottrell and J. R. Rice, Int. J. Fract. 16, 155 (1980).



Fig. 22. Branching motion of a crack in which the crack abruptly changes cleavage plane.

referred to these authors for an excellent discussion of the branching force, and for with the further literature on the subject.

The relation between K and k in the analysis leading to Eq. (16.4) yields again the complex number form of the shielding relations for Modes I and II:

$$\bar{K} = \bar{k} + \frac{\mu}{2i(1-\nu)} \sum_{j} \left( \frac{b_{j}}{\sqrt{2\pi\zeta_{j}}} + \frac{b_{j}}{\sqrt{2\pi\zeta_{j}}} + \frac{\pi \bar{b}(\zeta_{j} - \bar{\zeta}_{j})}{(2\pi\zeta_{j})^{3/2}} \right).$$
(16.7)

The force on the dislocation requires an evaluation of the residue at  $\zeta_j$ , and is much more complicated than in antiplane strain. Again, as in Eq. (15.7), there are there separate contributions to this force, which will be denoted

$$f_d = f_{Kd} + f_{d^2} + f_{dd^2}.$$
 (16.8)

The first term is linear in the reference dislocation b, and linear in K. It corresponds to the direct interaction between the crack and the dislocation. The second term is proportional to  $b^2$ , and represents the self-image term. Finally, the third term is proportional to  $bb_j$  and represents the dislocationidislocation interaction. These three terms will be addressed in turn.

The direct crack-dislocation force is

$$\vec{J}_{Kd} = \frac{1}{2i\sqrt{2\pi\zeta}} \left( Kb - \bar{K}\bar{b} + \frac{\bar{K}b(\zeta - \bar{\zeta})}{2\zeta} - \bar{K}b \right) - \frac{K\bar{b}}{2i\sqrt{2\pi\zeta}}.$$
 (16.9)

Since the distocations in question are edge in character, it is convenient to inswrite Eq. (16.9) in terms of a coordinate system rotated so the slip plane lies along: the real axis (Fig. 23). In this coordinate system

$$\bar{f}^{*p} = \bar{f}e^{ia}; \quad b^{*p} = be^{-ia}; \quad \text{etc.}$$
 (16.10)

 $b^{ap}$  by: definition is real, i.e.,  $b^{ap} = b_e$ , and equal to the edge component of the idislocation. In this coordinate system,

$$\tilde{f}_{1\,Kd}^{sp} = \frac{b_e}{2\sqrt{2\pi r}} \left( \frac{Ke^{i\alpha} - \bar{K}e^{-i\alpha}}{i} e^{i(\alpha - \theta/2)} + \bar{K}\sin\theta e^{i(2\alpha - 3\theta/2)} + i\bar{K}e^{i(2\alpha - \theta/2)} + iKe^{i\theta/2} \right).$$
(16.11)

Note that the  $\operatorname{Re}(\overline{f}^{\operatorname{sp}})$  is the slip force on the dislocation and  $-\operatorname{Im}(\overline{f}^{\operatorname{sp}})$  is the dimb konce.

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Fig. 23. Configuration of Mode-I and -II edge dislocation in slip-plane coordinates.

When the slip plane intersects the tip, then  $\alpha = \theta$ , and Eq. (16.11) simplifies to

$$\operatorname{Re}(\tilde{f}_{kd}^{sp}) = \frac{b_e}{2\sqrt{2\pi r}} [K_1 \sin\theta\cos\theta/2 + K_{ll}(2\cos3\theta/2 + \sin\theta\sin\theta/2)].$$
(16.12)

For future reference, inspection of the angular parts of this equation indicates that dislocations are likely to be more strongly affected by  $K_{\rm H}$  than by  $K_{\rm L}$ . For rough estimation, Eq. (16.12) gives a good picture of the force on dislocations in the deformation zone, because generally speaking, it is those dislocations whose slip planes roughly intersect the crack tip which do the shielding. After they are left behind in the wake, for instance, they have little interaction with the crack tip, and their prime interaction is with themselves and possibly with the open cleavage surface.

The second term in Eq. (16.8) is the self-image term quadratic in b, and is given by

$$\bar{f}_{d^2} = -\frac{\mu}{4\pi(1-\nu)} \left\{ \frac{b^2 \sqrt{\zeta}}{\zeta^{3/2}} \left[ 1 + \left(\frac{\bar{\zeta}}{\zeta}\right)^{1/2} \right] + \frac{b\bar{b}}{4} \left[ \frac{3}{\zeta} + \frac{1}{2\sqrt{\zeta}\bar{\zeta}} \left( 1 - \frac{\bar{\zeta}}{\zeta} \right) + \frac{3 - \sqrt{\zeta/\zeta}}{\sqrt{\zeta}(\sqrt{\zeta} + \sqrt{\zeta})} \right] - \frac{\bar{b}^2}{4\bar{\zeta}} \left[ 1 + \left(\frac{\bar{\zeta}}{\zeta}\right)^{1/2} \right] \right\}.$$
(16.13)

When slip-plane coordinates are used and  $\theta = \alpha$ , the result is

$$(\bar{f}_{d^2}^{sp})_{\rm hip} = -\mu |b^2|/4\pi (1-\nu)r, \qquad (16.14)$$

$$(\bar{f}_{d^{2}}^{sp})_{climb} = \frac{\mu b^{2} \tan{(\theta/2)(5+3\cos{\theta})}}{16\pi(1-\nu)r^{2}}.$$
 (16.15)

The result Eq. (16.14) was first given by Rice and Thomson,<sup>37</sup> and has the same form as in antiplane strain. That is, Eq. (16.14) is the same as the simple image force on a dislocation at a distance r from an infinite surface.

The third term in Eq. (16.8) is bilinear in  $bb_j$  and is the dislocationdislocation term. The general expression is

$$\frac{8\pi(1-\nu)}{\mu}\bar{f}_{dd'} = (bb_{j} + \bar{b}b_{j} + b\bar{b}_{j})\left\{\frac{1}{\xi_{j}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} + 1\right] + \frac{1}{\xi_{j}^{*}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} - 1\right]\right\} \\ - \bar{b}\bar{b}_{j}\left\{\frac{1}{\xi_{j}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} + 1\right] + \frac{1}{\xi_{j}^{*}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} - 1\right]\right\} \\ - 2b_{j}biy\left\{\frac{1}{\xi^{2}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} + 1\right] + \frac{1}{\xi^{*2}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} - 1\right]\right\} \\ + \frac{bb_{j}iy_{j}}{\xi^{2}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} + \left(\frac{\zeta}{\zeta_{j}}\right)^{1/2} + 2\right]$$
(16.16)  
$$- \left(\frac{(\bar{b}\bar{b}_{j} + b\bar{b}_{j})iy_{j}}{\xi^{*2}} + \frac{4b\bar{b}_{j}yy_{j}}{\xi^{*3}}\right)\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} + \left(\frac{\zeta}{\zeta_{j}}\right)^{1/2} - 2\right] \\ - \frac{\bar{b}b_{j}iy_{j}}{\xi^{*2}}\left[\left(\frac{\zeta_{j}}{\zeta}\right)^{1/2} + \left(\frac{\zeta}{\zeta_{j}}\right)^{1/2} - 2\right] - \frac{bb_{j}iy}{\zeta^{3/2}}\left(\frac{\sqrt{\zeta_{1}}}{\xi} + \frac{\sqrt{\zeta_{1}}}{\xi^{*}}\right) \\ + \frac{b\bar{b}_{j}yy_{j}}{\xi^{*2}}\left(\frac{1}{\sqrt{\zeta_{j}}} - \frac{\sqrt{\zeta_{j}}}{\zeta^{3/2}}\right),$$
  
$$\xi_{j} = \zeta - \zeta_{j}; \qquad \xi_{j}^{*} = \zeta - \bar{\zeta}_{j}; \qquad y = (\zeta - \bar{\zeta})/2i; \qquad y_{j} = (\zeta_{j} - \bar{\zeta}_{j})/2i.$$

This complicated expression is a bizarre example of how difficult it can become to solve boundary-value problems in elasticity for any but the simplest situations. The various distances,  $\xi$ ,  $\xi^*$ , etc., are diagrammed in Fig. 24.



Fig. 24. Diagram of the distances  $\xi_j$ ,  $\xi_j^*$ ,  $\tilde{\xi}_j$ , and  $\tilde{\xi}_j^+$  for a pair of dislocations at  $\zeta$  and  $\zeta_j$  for interpretation of Eq. (16.16).

## 17. THE WEDGE CASE

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When dislocations are in the elastic field of a wedge crack, then the equations for the potentials given in Part III, 11 apply. For the Mode I-II case, the results become quite complicated, and the reader is referred to the paper by Sinclair<sup>24</sup> for numerical results. In Mode III, when the dislocation is on the  $x_1$  axis, the results are (see Fig. 19).

$$f_{e} = 0, \qquad p \neq 2,$$

$$\bar{f}_{d} = \frac{\Lambda b}{\zeta^{1-q}} - \frac{\mu b^{2}}{4\pi\zeta} \frac{1}{1 + (\bar{\zeta}/\zeta)^{q}}, \qquad (17.1)$$

$$q = 1/p.$$

These results for the dislocation reduce to the slit crack when p = 2. The curious result is that  $f_e = 0$  when the wedge angle is finite. The analytic reason is that the singularity at the crack tip then differs from  $1/\sqrt{r}$ , and no residue exists. On the other hand, the wedge can certainly be extended, geometrically, into the medium, and when it does so, the external surfaces of the material extend, and work is done by the external stressing machines. So a paradox exists. The resolution is by means of the construction in Fig. 25, which shows that a self-similar translation of the wedge, in which its elastic stress field is rigidly translated with it, can only be produced by dislocation emission. That is,



Fig. 25. When a wedge is translated to the right, the arrows show the displacement necessary, and indicate an accumulation of strain at the tip and along the sides. Thus, self-similar translation of the wedge and strain field is impossible elastically. When dislocation emission is allowed, such translation is possible.

if the wedge is cut open at its tip, and the faces forced into the wedge shape, elastically, then the stress field is not translationally invariant as the process continues as required in the Eshelby theorem. On the other hand, after emission of dislocations from the tip, the stress field of the wedge does so translate (when the dislocations move away!). But dislocation emission generates nonzero incompatibility, and is therefore nonelastic. If the work done on the dislocations as they are emitted is included in the analysis, then the work done as they emerge from the external surfaces is just that done by the external stressing machines, which resolves the paradox. In other words, there is no elastic force on the wedge as it translates, but there is on the dislocations. Closely coupled to this distinction between cracks and wedges is the fact that a Mode-I wedge does not disappear when the external stress is removed, even though the stress singularity does. By contrast, the cleavage crack, of course, has the basic property that, when the external stress is removed, the atom bonds zip together again and the crack disappears. Thus, the wedge is, fundamentally, a void (made by punching out dislocation loops or agglomeration of vacancies), whereas cleavage cracks are a logically distinct class of crystal lattice defect. This analytically derived distinction between cleavage cracks and wedges is, of course, intimately connected with the physical consequences for toughness to be discussed in later sections. (The dislocations in this discussion are, of course, "real" dislocations, as distinct from the virtual or "crack" dislocations introduced by Friedel and discussed in Part II,5.)

### 18. THE J INTEGRAL

Equation (14.8) as applied to cracks was derived independently of Eshelby by Rice, 30-32 who called the right-hand side of Eq. (14.8) the J integral. J is used extensively in the fracture mechanics field for the analysis of fracture in plastic materials. Unlike our approach, which addresses plasticity in terms of the individual dislocations which are the seat of crystal placticity, J is calculated using continuum plasticity theory under the assumption that the medium obeys a nonlinear stress-strain law, which is a single-valued function of strain. From the definition of the strain-energy function, Eq. (14.11), W is then no longer a quadratic function of strain.

$$W = \frac{1}{2} c_{(RI} \varepsilon_{IJ} \varepsilon_{Le_{J}} \tag{18.1}$$

but a more general nonlinear function of the strain. If this more general stressstrain law is a unique single-valued function of strain, then Eq. (14.12) is still valid, and the integral in Eq. (14.10) is still zero. Thus J is path independent.

The difference between J and f as we have used it is that in J there are no singularities representing the dislocations of the plastic zone, only a nonlinear stress-strain "constitutive law." Thus, unlike f, the contour path for J can be

shrunk through the deformation zone to the crack tip itself, for all of which contours, the value is an invariant. Further, outside the deformation zone, J is exactly the same as calculated for our f, and in this case, from Eq. (15.10).

$$J_{\rm III} = \text{Re}(f_{\rm ini}) = K_{\rm III}^2 / 2\mu.$$
(18.2)

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Similar equations follow for Modes I and II.

$$J_{\rm E,H} = \operatorname{Rc}(f_{\rm int}) = [(1 - v^2)/E](K_1^2 + K_H^2). \tag{18.3}$$

Note that we have followed tradition and defined J for the  $x_1$  component of the force only.

Equations (18.2) and (18.3) follow only when a K field can be defined outside the deformation zone. That is, the boundaries of the specimen must be far away from the edge of the plastic zone surrounding the crack on a scale based on the size of the deformation zone. This case is called the "small-scale yielding" approximation. The major usefulness for J comes from its use when the small-scale yielding approximation is not valid (see Fig. 26). In this latter case, of course, J is still calculable by Eq. (14.8) even though no K field can be inferred. But the relation to the force has a less clear meaning—in our terms,



Fig. 26. Small-scale yielding. In (a), the deformation zone surrounding a crack (shown shaded) is small compared to all physical dimensions of crack size and specimen size. A K field outside the deformation zone is well defined. In (b), the deformation zone overlaps the specimen surfaces, and no K field can be defined at large distances from the crack. Nevertheless, J can be calculated in the latter case and is contour invariant.

the dislocations of the deformation zone may disappear in the boundary when the configuration is displaced if the deformation zone overlaps the boundary, for example.

The great value of J is associated with the fact that it is a characterizing parameter for a crack in a given material, and critical values of J can be measured for cracks at which catastrophic failure occurs,  $J_c$ . From its derivation,  $J_c$  is a parameter which depends only on the material properties such as yield stress, work hardening, etc., and can be used as a measure of the susceptibility of a material to failure under various conditions of stress and crack size. Moreover,  $J_c$  is a parameter which can be measured for specimens where the small-scale yielding assumption is no longer valid. Although there is some uncertainty about its physical meaning in this case, one would roughly expect from its contour invariance that the conditions at the crack tip which cause crack growth should continue to be approximately inferred by  $J_c$  even when not in small-scale yielding. Indeed, empirical explorations have shown that  $J_c$  is in fact an excellent fracture criterion in the large-scale or general yielding case as well as for small-scale yielding. (See the engineering references below.)

A more serious problem arises when a crack is stressed to the critical level and actually moved. As the crack moves, it leaves behind in its wake material which has gone through a stress cycle of loading followed by release. The J formalism is only valid if the release of stress follows the reversible stressstrain law used in deriving W in Eq. (14.11). Unfortunately, real materials exhibit considerable hysteresis if they are cycled into their plastic regimes, so that the J formalism is not valid for a crack which begins to move, and of course, most certainly not for one in something approaching steady-state or dynamic conditions. (Eshelby has described this condition on J in the classic words that the  $J_c$  concept is valid "so long as one does not call the material's bluff" by unloading it!) A great deal of work has been done to explore the practical limits of this difficulty for engineering purposes, and the limitations do not impose important constraints for crack initiation measurements and, surprisingly, not even for fatigue growth.41.42 The reader is referred to the various volumes of the ASTM series for the details of the engineering applications, especially the article by Begley and Landes<sup>43</sup> and the book edited by Campbell et al.44

42 H. Heitmann, H. Vehoff, and P. Neumann, Fatigue Eng. Matr. Str., in press (1986).

<sup>43</sup> J. Begley and J. Landes, Fracture toughness ASTM Spec. Tech. Publ. 560, p. 186; see other articles in this publication.

<sup>44</sup> J. Campbell, W. Gerberich, and J. Underwood, "Application of Fracture Mechanics for Selection of Metallic Structural Materials." ASM, Metals Park, Ohio, 1982.

<sup>41</sup> C. Wutherichs, Int. J. Fract. 20, R35 (1982).

For the purposes of this article, however, J and the continuum plastic approach have important limitations.45 Perhaps the most important reason follows from a crucial theorem of Rice, 32.46 which states that if the stress field saturates near a crack tip, as it must in a plastic theory with a realistic finite plastic yield condition (which may incorporate strain hardening), then as the crack moves forward, all the energy supplied by the external loading machine is absorbed by the deforming region, and none is left over to provide energy to open the surface. We will return to this issue in Part VII, but this theorem is a fatal blow to the attempt to understand the conditions under which a crack will open (what we will call the fracture criterion) on the continuum level, because the energy supplied to open the bonds at the crack tip is the crucial event in the entire crack growth process. We will show that it is the local k which is important in this connection. That is, unlike J, which is a complete invariant.  $\overline{f}$  gives a different value when the contour only encloses the local crack tip than when it encloses all the dislocations in the deformation zone, and it is this distinction which will allow a microscopic physical picture of the cracking process to be constructed.

#### **19. THE GRIFFITH RELATIONS**

This section will be concluded with a review of the classic work of Griffith on the equilibrium of cracks in brittle materials.<sup>47</sup> This is the simplest example of crack equilibrium, a subject to which we return in Part VII.

It will be assumed that the crack of Fig. 16b is loaded in Mode I. Then, since there are no dislocations present, the elastic force on the crack, Eqs. (16.5) and (16.6), is

$$f_{\rm c} = \frac{(1-\nu)}{2\mu} K_1^2. \tag{19.1}$$

Opposing this elastic force are resistive forces to crack opening provided by the material. In later sections, a variety of such forces will be considered, but there is always one contribution for a Mode-I crack, namely the simple surface tension of the opening surfaces at the crack tip. Working by simple analog to a soap bubble-like surface tension operating at the crack tip and neglecting for the moment the complexities of surface tension in a solid, the opposing force exerted on the crack by the crystal is simply

$$f_{\rm errs} = -2\gamma. \tag{19.2}$$

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<sup>45</sup> Fracture mechanics in design and service: A Royal Society discussion organized by H. Ford, P. Hirsch, J. Knott, A. Wells, and J. Williams. *Philos. Trans. R. Soc. London Ser. A* 299, 3 (1981).

46 J. Rice, Proc. Int. Conf. Fract. Sendai 1, p. 309 (1966).

47 A. A. Griffith, Philos. Trans. R. Soc. London Ser. A 221, 163 (1920).

(Note there are two surfaces presented to the crack tip.)

When the elastic forces and surface tension forces are in balance, then the point of equilibrium is given by the critical value of K,

$$K_{\rm ic} = 2\sqrt{\gamma\mu/(1-\nu)}.$$
 (19.3)

This equation is often called the Griffith relation, although it is not in the form given by him, since the stress intensity factor was introduced much later.

The point of equilibrium is actually unstable for the most usual form of crack loading (Problem 1), a fact most easily seen by working with the energy of the system. For Mode 1, from Eqs. (9.10) and (18.4) the energy of the system with the double-ended crack of Fig. 16b is given by

$$U=2\int_0^{\infty}(f_c+2\gamma)\,da$$

$$[\pi F^2 a^2 (1-\nu)/2\mu] + 4\gamma a. \tag{19.4}$$

This expression represents an inverted parabola as a function of the crack length, a, with its maximum at the Griffith stress,  $\sigma_G$ ,

$$\sigma_{\rm G} = 2\sqrt{\gamma \mu/\pi a(1-\nu)}. \tag{19.5}$$

This is the equation derived by Griffith<sup>47</sup> (as corrected — see Goodier<sup>19</sup>). With the assumed loading geometry, the crack is in unstable equilibrium at the Griffith point. With other forms of loading the specimen, for example by using a wedge at the crack mouth with a point-function opening force exerted at the mouth, the crack can be stable at the Griffith point. For these reasons, Eq. (19.3) is a more general and satisfactory way of expressing the crack equilibrium, because it is independent of the loading geometry. The reader will note that Eqs. (19.3) and (19.5) are equivalent through Eq. (9.10).

In the usual derivation of the Griffith equation (and in his original paper) a careful distinction is made between the elastic energy of the medium and the potential energy change of the external stressing machine. This subtlety is included in the Eshelby derivation of the force on the crack. Thus,  $f_c$  is not the derivative of the internal energy of the material with respect to crack position, but the derivative of the elastic energy of the total system, including energy changes of the external stressing machines, with respect to crack position.

The instability at the Griffith value is the physical reason why fracture is often catastrophic when a critical stress is reached on a crack and, of course, is the physical basis for the enormous practical importance of fracture control in actual materials. The instability in the other direction, i.e., crack closure, is not normally observed (except in polymers!) because the surfaces, once open, are subject to oxide formation, deformation, etc., so that crack closure with exact registry is difficult to effect. It is observed in brittle solids when sufficient care is taken, however. (See Fig. 9b.)

# V. Atomic Structure of Cracks

20. INTRODUCTION

The discrete atomic nature of matter leads to chemical and other bondlir g effects at crack tips which generally go beyond simple continuum concepts. will thus be necessary to develop descriptions of cracks in lattices. This gamerall subject falls into two subheadings, the problems associated with clearage (including the chemical effects) and the problems associated with the breakdown of the crack with emission of a dislocation. These two subjects will be treated consecutively in this and the following section. The mathematical framework will, however, be dealt with here. Although this discussion and I address the properties of the ideal brittle crack, the ideas presented will be applicable to cracks shielded by dislocations in more general circumstances.

## 21. LATTICE STATICS

The mathematics of lattice statics for describing defects in lattices that recently been reviewed by Bullough and Tewary.<sup>44</sup> This method yields such a simple and accessible approach to the cracked lattice, that we will use at to discuss cracks in a simple 2D lattice in some detail. The discussion is based on the papers of Hsieh and Thomson, 49 Esterling, 50 and Thomson and Fuller. 511

We imagine a lattice as shown in Fig. 3, which is bound bymearest-neighbor forces. The crack is defined by cutting a finite number (2N +++ 3) of the bounds crossing the cleavage plane. An external force,  $F_0$ , is assumed to act on the two atoms at the center of the crack to hold the crack open, again as shown in Fig. 3. It is assumed that all the atoms of the crystal are bondled by springs, 150 that the system as a whole responds in a strictly linear manner to the imposition of the external force, Fo. Finally, it is assumed that arbitrary bonding forces, f, are applied to the pair of atoms at each endeof the cut, which for the moment will be viewed as "external" forces. The response of the system can then be written in the form

$$\mathbf{U}_i = \sum \vec{G}_{ij} \mathbf{F}_j. \qquad | (2 \mathbf{J}_i) |$$

 $U_i$  is the displacement of the *j*th lattice point, and  $\tilde{G}$  is the Green's tensor if  $u_i$ 

48 R. Bullough and V. K. Tewary, "Dislocations in Solids" (F.R. N. Navamp, ed.)/ Voll 2, pull. North Holland Publ., Amsterdam, 1979.

49 C. Hsich and R. Thomson, J. Appl. Phys. 44, 2051 (1973).

<sup>50</sup> D. Esterling, J. Appl. Phys. 47, 486 (1976).

31 R. Thomson and E. Fuller, in "Fracture Mechanics in Ceramics" (R. Bradtm al., eds.), Plenna,

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the cracked lattice.  $\ddot{G}$  is a function of N, the crystal structure, and the direction of the cleavage plane in the lattice. u and F are vectors. Equation (21.1) is a general lattice equation, and can be applied to any lattice or direction of crack. But in order to develop some simple illustrative results, we will restrict the following discussion to simple cubic lattices, with  $\mathbf{u}$  and  $\mathbf{F}$  in the  $x_2$  direction, so that these quantities become simple scalars. Then, because of symmetry, with only the forces  $F_0$  on the central pair and  $-f_N$  on the atoms at the tip, when  $N \gg 1$ , the two equations from the set of Eq. (21.1) most important to us are those giving the displacement of the center of the crack,  $u_0$ , and the displacement at the tip  $u_N$ . Thus

$$u_0 = G_{00}F_0 - 2G_{0N}f_N,$$
  

$$u_N = G_{0N}F_0 - G_{NN}f_N,$$
(21.2)

the distinction of capital and lowercase between  $F_0$  and  $f_N$  is made to emphasize the point that  $F_0$  is a "real" external force, while  $f_N$  will ultimately be interpreted as an atomic bond force.

The general formalism of Bullough and Tewary<sup>48</sup> for lattices has to be modified to obtain the relevant Green's tensor for the crack. In brief, for the crack, the G is obtained by calculating the displacement from the perfect lattice Green's tensor due to a unit force, when fictitious forces are simultaneously applied on the cleavage plane to annihilate the bonds there. The result is the cracked lattice Green's function, and details for finding it will be found in Hsich and Thomson.<sup>49</sup> For present purposes, the coefficients,  $G_{00}$ , and  $G_{0N}$ and  $G_{NN}$  are simply taken as given constants.

The character of the crack solution is then easily seen by inspection of the first of Eqs. (21.2) when f is set to zero, viz.  $u_0 = G_{00}F_0$ . The displacement as a function of  $F_0$  is simply a straight line with slope  $G_{00}$ , where the slope is a function of N. For different values of N, the solution is then a manifold, as shown in Fig. 27. If the force law is assumed to possess a critical range, as shown in Fig. 29a, then there exists a maximum value of displacement  $u_0$  when the bond at the tip reaches the critical displacement. Thus, the portion of the line in Fig. 27 larger than this maximum value (above the upper limit curve) is not an allowed part of the solution. Likewise, when  $F_0$  is decreased, there comes a point where the last open bonds on the cleavage surface at the tip snap back together, and again, portions of the line less than this value (below the lower limit curve) do not represent a solution. Thus, the crack "solution" for different values of crack length is the set of lines between the limit curves of Fig. 27. This solution shows that for a given value of crack length, the crack is stable over a range of external forces, and for a given  $F_0$ , a number of crack lengths have stable solutions. This result is contrary to the continuum solution, Eq. (19.4), where there is only a single stable solution (crack length) at



FIG. 27. Solution of Eq. (21.2). A family of compliance curves is generated for various values of crack length N. The curves are limited at a maximum displacement by the bond strength at the tip, and at a minimum displacement by reconnection of the first broken bond at the tip. At the maximum displacement for N, the solution snaps back to N + 1 at the minimum, as shown by the dotted lines, provided F can be varied at the same time.

the maximum of a parabola. [The loading conditions of Fig. 3 and for Eq. (19.4) are not the same, but the result is still the same—continuum theory using the loading system of Fig. 3 yields only a unique crack length for any external load,  $F_0$ .] When nonlinear bonding forces  $f_N$  are postulated at the tips of the crack, then the straight lines of Fig. 27 become the continuous curve shown schematically for a single branch in Fig. 28.

The multiple crack solutions depicted by Fig. 27 are separated by energy barriers, explained as follows. In Fig. 28, the line for constant  $F_0$  crosses the curve at three points. The energy necessary to move from point 1 to point 2 is given by the expression

$$\Delta E_{12} = \int_{1}^{2} F_0(u_0) du_0 - F_0 \Delta u_0. \qquad (21.3)$$

The first term is the change in internal energy of the system, and the second is the change in potential energy of the external driving system.  $\Delta E_{12}$  is the total energy change.  $\Delta E_{12}$  is thus the cross-hatched area shown in Fig. 28 from point 1 to point 2, and is a positive energy. To go from 2 to 3 is a negative energy. Thus, states 1 and 3 are stable states, and state 2 is a saddle point in configuration space between the two stable states.

This energy is easily calculated if the force law is known, by reference to Eq. (21.2). In this equation, the forces  $f_N$  are now assumed to be the actual nonlinear bonding forces exerted by the atoms according to some specified force law, Fig. 29. Since  $f_N = f_N(u_N)$  is a nonlinear function of  $u_N$ , the set of



Fig. 28. Crack solution for nonlinear forces for N and N + 1. For a given F several discrete solutions are possible. Positions 1 and 3 are stable. Position 2 is unstable. The cross-hatched areas correspond to trapping barriers. That from 1 to 2 is a forward barrier and that from 3 to 2 is a reverse barrier.



FIG. 29. Bond forces f. A variety of bond forces are discussed. In the left-hand part, the force is a snapping spring. In the right-hand part, a more realistic nonlinear force is shown.

equations (21.2) become a pair of coupled nonlinear equations for the displacements  $u_0$  and  $u_N$  in terms of the independent variable  $F_0$ . The constants G are still the linear lattice Green's tensor, however. If  $f_N$  is eliminated from Eq. (21.2), then after taking differentials.

$$du_0 = \frac{2 G_{0N}}{G_{NN}} du_N + 2 G_{0N} \left( \frac{G_{00}}{2 G_{0N}} - \frac{G_{N0}}{G_{NN}} \right) dF.$$
(21.4)

Here and later we drop the subscript from F and f because no confusion is possible. Substitution of this expression into Eq. (21.3) yields

$$\Delta E_{12} = 2 \int_{1}^{2} \frac{G_{0N}}{G_{NN}} F \, du_{N} - F \, \Delta u_{0}. \tag{21.5}$$

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the term  $\int_{1}^{2} F dF$  is dropped from Eq. (21.5) because states 1 and 2 have the same value of F. Substituting for F from Eq. (21.2) and for  $\Delta u_0$  from Eq. (21.4),

$$\Delta E = 2 \int_{1}^{2} f(u_{N}) du_{N} + \frac{1}{G_{NN}} \Delta(u_{N}^{2}) - \frac{2 G_{0N}}{G_{NN}} \Delta u_{N}. \qquad (21.6)$$

In this equation, f(u) is explicitly the atomic bond function, and is given by the functional form illustrated in Fig. 29. Equation (21.6) exhibits an important theorem for all nonlinear atomic processes at the tip, when the nonlinear process is limited to only one atom, which we will call the decomposition theorem. The activation energy  $\Delta E_{12}$  is composed of three additive parts. The first is the energy change in the chemical bond at the tip, and is the only term which can reflect the influence of external chemistry. The second is the change in the linear lattice, which is a simple quadratic function of the displacement change at the tip (or alternatively, displacement at the point of force application). The third is the change in the external machinery potential energy which is a negative linear term. The last two terms depend only upon the linear properties of the bulk material. This simple decomposition theorem can be used to deal qualitatively with complicated chemical interactions at the crack tip, even when the nonlinearity is not strictly limited to a single bond. The decomposition theorem is graphically depicted in Fig. 30.



Fig. 30. Diagrams illustrating the decomposition theorem. The broad displaced parabola is composed of the second and third terms of Eq. (21.6). The atomic-bond function is displayed in each of three cases superimposed on the parabola. The resultant is the dotted curve. In (a) the bond function is weak and not near the parabola minimum; no activation energy. In (b), the bond is strong, and has its maximum slope close to the parabola minimum; activation energy. In (c), an additional chemical activation energy is present, which adds a large bump to the total activation energy.

The model above has been pursued more quantitatively by Thomson and Fuller<sup>51</sup> to explore the sensitivity of the energy barriers to force-law form, and to explore the stress dependence of the barriers. In general, the result is that an extreme snapping force law like Fig. 29a leads to a maximum trapping, compared to the softer law of Fig. 29b. This result and that of other discrete crack theories, suggest that for realistic force laws in materials, the 2D energy barrier will lead to a trapping stress range which will be small compared to the Griffith stress. The energy dependence of the energy barriers is found to depend on the type of force law, and

$$E_{12} \propto (k - k_c)^n$$

$$n = \begin{cases} 2, & \text{snapping bond (Fig. 29a),} \\ \frac{3}{2}, & \text{inverted parabola.} \end{cases}$$
(21.7)

 $k_r$  is a constant, and is the value of k when dynamic cleavage occurs. The 2D mathematics above does not account for the fact that the real crack will make use of its third degree of freedom in moving from one atom row to the next. In particular, just as for dislocations, any crack limited by the lattice barriers will traverse the barriers by nucleation of a double kink of finite length, so the energy to cross traversing the barrier will be finite. Such kinks were proposed by Hsieh and Thomson,<sup>49</sup> and have been discussed semiquantitatively by Esterling,<sup>50</sup> Sinclair<sup>52</sup> for simulated Si, and by Lin and Hirth<sup>53</sup> in a quasicontinuum model.

The only other fully published work with the lattice statics approach is that by Esterling, 50 who explored a variety of force laws at the tip, and who first pointed out that nonsnapping force laws were accessible with the latticestatics approach. He also made some estimates of kink configuration in a quasi-3D calculation. All such work done by the authors, 49-51 however, was performed in simple square lattices, and was limited to nonlinear forces restricted to the tip bonds. As such, this work is only of very rough qualitative significance. However, the analysis is actually entirely general, and in principle can be applied to any lattice structure and to any number of nonlinear forces at the tip. For other lattices, the Green's tensor would be more difficult to calculate than for the square lattices, but the strategy outlined in Hsieh and Thomson<sup>49</sup> for generating the Green's tensor is applicable using the generat theory given in Bullough and Tewary.48 In addition, if more than one nonlinear bond is contemplated at the tip, then additional terms,  $f_j$  and  $u_j$  at the tip, must be included in Eq. (21.2). Counting the displacement  $u_0$ , Eq. (21.2) becomes a set of (L + 1) equations for  $u_0, u_N, u_{N+1}, \dots, u_{N+L}$  in terms of  $F_0$ ,

52 J. Sinclair, Philos. May. 31, 647 (1975).

51 I. H. Lin and J. P. Hirth, J. Mater. Sci. 17, 447 (1982).

 $f_{w}(u_{n})$ , etc. This is now a set of (L + 1) nonlinear equations which will require numerical techniques to solve, but poses no further analytic difficulties. Thus, the extended fattice statics approach as outlined here is a very powerful method for obtaining general quantitative results. Once the Green's tensor has been calculated for a given lattice (for a given crack length), then the generalization of Eq. (21.2) can be solved for any arbitrary set of force laws (or chemical interactions), and much insight into the various fracture configurations could be gained. It is to be emphasized that the analysis is not in any way limited by considerations of whether the set of atoms in the discrete lattice is large enough (because it is co), or by considerations about boundary conditions between some internal discrete enclave and an outer infinite crystal, because there is no such arbitrary boundary in the problem. Sinclair<sup>54</sup> has reported some initial results on such a program relating to the problem of dislocation emission, but this work is still in progress at the time of writing.

### 22. DISCRETE-ENCLAVE METHOD

A second method for studying the atomic configurations of cracks embeds a finite discrete set of atoms within a surrounding continuum. The comfiguration is then found numerically by successive approximation of a selfconsistent displacement field in the discrete set and in the continuum. This method has a long history for all sorts of defect calculations, and has been used to simulate cracks in real materials. The first such attempts were made by Gehlen and Kanninen<sup>55</sup> using the Johnson<sup>56</sup> potential for iron, and these authors in various combinations with A. Markworth and J. Hirth gradually improved the early computer model over a number of years, in part with a continuum Green's function technique of J. Hirth<sup>57</sup> so that a flexible boundary is allowed between the continuum and discrete regions. In addition, an attempt was made to model the effects of hydrogen on the configuration. Results of this work, together with references to prior work, are given in the paper by Markworth et al. 38 The reader is also referred to the paper by Sinclair et al. 59 for details on the flexible boundary method (Flex II) as it has been developed for simulation calculations using two embedded regions inside an

34 J. Sinclair, to be published (1986).

- 55 P. C. Gehlen and M. F. Kanninen, in "Inelastic Behavior of Solids" (M. Kanninen et al., eds.), p. 586. McGraw-Hill, New York, 1970.
- <sup>56</sup> R. A. Johnson, Phys. Rev. 134, A 1329 (1964).
- 17 J. Hirth, Scripta Metall. 6, 535 (1972).
- <sup>58</sup> A. J. Markworth, M. F. Kanninen, and P. C. Gehlen, Proc. Int. Conf. Stress Corrosion Cracking, France June 12 (1973); see also, P. C. Gehlen, G. Hahn, and M. F. Kanninen, Scripta Metall, 6. 1087 (1972)
- <sup>19</sup> J. Sinclair, P. C. Gehlen, R. G. Hoagland, and J. P. Hirth, J. Appl. Phys. 49, 3890 (1978).

outer continuum. In part, this work has been aimed at simulating cleavage in iron and Fe/H, but it has also been used to study the dislocation emission problems, as discussed in the next section.

Sinclair<sup>52</sup> has used Flex II to simulate a crack in Si, using a directed-bond noncentral force, and has studied how the lattice trapping varies with choice of the radial part of the force law. In addition, he has estimated the kink motion and formation energies for Si with these laws, and finds that the kink motion energy is in the range 0.01 eV, and that the kink pair-formation energy is of the order 0.1 eV. The estimate of formation energy, however, is very crude, and based on a quasicontinuum string model of the crack. The interesting conclusion from this work, however, is that even in this most favorable case. the lattice trapping barriers are estimated to be small, though the actual numbers involved must be considered very rough estimates for the 3D quantities because of uncertainty in the force law,

Most recent work with this method has been an extensive study of simulated Fe with the Johnson potential and simulated Cu with the Morse potential by de Cellis et al.,60 with the intent to study the dislocation emission question of Part VI. The new mathematical development in this work is to derive a boundary condition between the discrete enclave and the continuum which is sufficiently flexible as to allow a dislocation to penetrate it. The iron cleavage plane was found to be {100}, and unlike the earlier work of the Battelle group, the critical k for cleavage is essentially the Griffith value. Other points discussed by these authors are the effect of isotropic/anisotropic elastic solutions in the continuum, and the effect of size of discrete enclave on the accuracy of the results.

Mullins<sup>61</sup> has also recently analyzed simulated iron with the Johnson potential to study dislocation emission and crack branching under mixed loading, with results to be discussed in Part VI.

#### 23. MOLECULAR DYNAMICS

Straightforward molecular dynamics has been applied to the crack problem by Ashurst and Hoover<sup>62</sup> and more recently in a series of papers by Paskin, Dienes, and collaborators.<sup>63-66</sup> In these calculations, 2D simulations are

- <sup>63</sup> A. Paskin, D. K. Som, and G. J. Dienes, Acta Metall. 31, 1253, 1841 (1983).
- 64 A. Paskin, K. Sieradsky, D. Som, and G. J. Dienes, Acta Metall, 30, 1781 (1982).

65

<sup>&</sup>lt;sup>60</sup> B. de Cellis, A. Argon, and S. Yip, J. Appl. Phys. 54, 4864 (1983).

<sup>&</sup>lt;sup>61</sup> M. Mullins, Int. J. Fract. 24, 189 (1984).

<sup>62</sup> W. T. Ashurst and W. G. Hoover, Phys. Rev. 1314, 1465 (1976).

<sup>45</sup> A. Paskin, D. K. Som, and G. J. Dienes, J. Phys. C 14, L171 (1981).

<sup>&</sup>lt;sup>46</sup> G. J. Dienes and A. Paskin in "Atomics of Fracture" (R. Latanision and J. Pickens, eds.), p. 671. Plenum, New York, 1983.

made with the largest number of atoms which are practicable in the computer  $(\sim 10^4)$ . The Lennard-Jones 6/12 power-law potential, truncated to include only the nearest neighbors, is assumed. Such a force law does not simu ale any particular material, but these authors have very astutely used the model to study a variety of general phenomena to be expected at the crack tip, and as a test bed for investigating the limit of applicability of quasicontinuum calculations. It has also proved possible for these authors to study both static and dynamically moving cracks by varying the external load. The results principally relate to dislocation emission effects, which are the subject of Part VI.

# 24. FORCE LAWS FOR DEFECT CALCULATIONS

Clearly, the calculations of crack structure depend in a crucial way on the validity of the force laws which are used. In ionic crystals, the Born-Mlayer type of theory can lead to defect calculations for the simple ionic materials possessing a fair degree of accuracy.<sup>67</sup> No crack calculations have been made in those materials, however, because the potential is long ranged, and this would lead to special problems with present techniques.

In the case of the simple metals, pseudopotentials have been used extensively for defect calculations.68 However, pseudopotentials in their standard form require that the volume change be small, and stacking faults are the only defects where the dilatation distortion is truly negligible. Since the crack involves an incipient surface, there is no hope that standard pseudopotentials can yield suitable force laws for crack calculations.

Another approach which has been used is the molecular cluster quantum chemistry approach. For example, charge distributions have been calculated for small clusters intended to simulate the vicinity of an impurity on a grain boundary, which are then used to rationalize what types of atoms will weaken or strengthen a boundary.<sup>69</sup> But the number of atoms needed to simulate the properties of a crack are well beyond current capabilities.

A third approach is completely heuristic, in which a spline or other function is constructed which is consistent with known material properties.48 The Johnson potential<sup>36</sup> for iron is such an example. However, there is no reason to believe that such an approach can yield any more information than is fed into it, so far as making predictions for a particular material is concerned.

Thus, the crack poses the same challenge as any defect, to calculate the absolute energy of a configuration from first principles, which is still one of the

most difficult things to do in theoretical condensed matter physics. But it also goes one step further, and adds a highly distorted surface, where the perturbation of the lattice (the volume-dependent term) is not weak. Hence, the crack is likely to be the last defect for which reasonable force laws can be obtained

In the opinion of the author, interesting progress is being made on two fronts. In the first, the tight-binding method has recently attracted considerable interest for calculating defect structures, and has the advantage that noncentral forces can be derived for the d shells. 70

The second approach has been an intensive effort by Barnett and Landman<sup>71</sup> to calculate the configuration of a surface in the simple metals. The result is a set of pair potentials which are structure dependent. Unfortunately, the volume- and structure-dependent effects are not always small.

Where do we stand? Clearly, for the near term, there is not likely to be a firstprinciples calculation of a crack tip. The best we are likely to have is some guidance from theory on general rules about what the "force laws" are like, and how to use them in a qualitative sense. But the crack will probably be the last defect for which a configuration calculation will be attempted which represents an actual solid. Thus, we are left only with the simulation of the general properties of cracks, and the rationalization of findings in terms of "green thumb" chemistry. But these efforts, as already shown by the work of Paskin et al., and Michalske and Freiman (see Part V,26) are likely to be very fruitful in terms of physical and chemical insight, until more quantitative help is available from first principles.

## 25. CHEMICAL KINETICS

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The general results above which show that discrete atomic effects at crack tips lead to energy barriers to crack motion are important for the interpretation of a variety of kinetic effects of fracture. Although, strictly speaking, the mathematical model in Part V,21 only addressed pure lattice effects, the discussion of the decomposition theorem in Fig. 30 shows that external chemical agents which can affect the bond breaking will conform to the same general conceptual framework. Likewise, although the barriers described above were those generated by the discreteness of the lattice, chemical attack at the tip will be discrete in the same way. Furthermore, it is a common occurrence for chemical reactions in the gas phase to have energy barriers to

<sup>67</sup> M. P. Tosi, Solid State Phys. 16, 1 (1964).

<sup>\*\*</sup> D. Esterling, Comments Solid State Phys. 9, 105 (1979).

<sup>\*\*</sup> C. Briant and R. P. Messmer, J. Phys. Collog. 43, 255 (1982).

<sup>78</sup> D. G. Pettifor, in "Atomistics of Fracture" (R. Latanision and J. Pickens, eds.), p. 281. Plenum, <sup>14</sup> R. N. Barnett and U. Landman, Phys. Rev. Lett. 51, 1359 (1983).



Fig. 31. Modified Griffith energy function. The smooth parabolic curve corresponding to Eq. (19.4) (----), becomes a "dinosaur back" function. The trapping occurs over the range  $\Delta N$  about the central maximum.

the reaction, and the highly constrained region of the crack tip will certainly enhance this possibility. Thus, barriers of one kind or another can be expected to show up for crack growth near the Griffith stress. Figure 31 is a schematic drawing of the modification which the energy barriers make in the continuum energy function, Eq. (19.4).

Physically, the energy barriers will give rise to a thermally activated crack growth (or, according to theory, to regression) near the Griffith point. Therate of jumping the barriers according to chemical reaction rate theory is<sup>71</sup>

$$v^{\bullet} = \frac{k_{\rm B}T}{h} \frac{Z^{\bullet}}{Z} = \left(\prod_{i=1}^{N} v_i / \prod_{i=2}^{N} v_i^{\bullet}\right) e^{-E_{12}/k_{\rm B}T}$$
(25.1)

Here the \* represents the 3D saddle configuration, Z is the partition sum,  $y_i$  is a frequency of the system, and  $E_{12}$  is the energy of the double kink. In the activated state, there is one fewer vibration frequency than in the stable state. When chemical reactions are taking place, the pre-exponential is modified from that of the simple lattice by incorporation of the appropriate partition sums for the gaseous and adsorbed chemical species.<sup>72</sup> The activation energy (even that for a 3D kink pair), should show the salient features of the 2D calculations, such as its k dependence.

When forward rates of motion for the crack equal the reverse rate, a condition for equilibrium between two stable states, 1 and 3, can be written

$$v_{13} = v_{31}$$
, or  $Z(1) = Z(3)$ , (25.2)

22 R. Thomson, J. Mater. Sci. 15, 1014 (1980).

which, in terms of the standard expressions relating the partition sums to the free energy F, becomes equivalent to F(1) = F(3).

This general condition for equilibrium does not mean that the rates are equal when the forward barrier in Fig. 28 or 31 is equal to the reverse barrier, because the states 1 and 3 are not equivalent states. State 3 differs from 1 by the addition (int 2D) of one surface pair. Thus, the vibration structure of the crystal with one additional surface pair is different from the initial state, and entropy contributions must be counted in setting up the free energy balance, F(1) = IF(3). Hence, at  $T \neq 0$ , there are subtle differences between forward and ireverse barriers. Similar results are, of course, valid in the case of chemical adsorption/during crack growth.

When the microscopic analysis is translated into the appropriate thermodymantic and mechanical variables, it can be shown<sup>72</sup> that F(1) = F(3) leads to the general law

$$f = 2\gamma, \tag{25.3}$$

where fishthe force on the crack derived in Part IV.  $\gamma$  is the temperatureindependent surface energy as defined by Gibbs. This equation remains valid in the case of ichemical interactions at the crack tip, and  $\gamma$  in that case depends in the istandard, way on the surface coverage of the external chemical species. Equation (25.3) was first suggested by Petch and Stables<sup>73,74</sup> on thermodynamic grounds for hydrogen embrittlement in Fe.

Mun interesting question arises when internal chemistry is combined with external chemistry, for example when a crack runs down a grain boundary with a iconcentration of solute impurity. If the initial grain boundary distribution is in thermal equilibrium with the dispersed impurity in the bulk solid, then, is the crack opens, the solute on the newly opened cleavage surface will usually not have time to come into equilibrium with the internal solute distributions. This problem has been analyzed in terms of a constrained equilibrium by Hirth and Rice,<sup>75</sup> with the result that when such a grain boundary opens, the y criterion is modified to be

$$\gamma \rightarrow \gamma - \frac{1}{2} \gamma_{GB} \tag{25.4}$$

where,  $\gamma_{\text{GHB}}$  is calculated for the boundary covered in such a way as to be consistent with the diffusion off the boundary which will be possible under the circumstances. That is, the energy and vibration entropy will be of the appropriately specified covered surface.

73 N. J. Petchiand P. Stables, Nature (London) 160, 842 (1952).

<sup>94</sup> N. J. Pelich, Philos. Mag. 1, 331 (1956).

3<sup>9</sup> J.IP. Hinth and J. Rice, Metall. Trans. A 11, 1501 (1980).

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# 26. SLOW-CRACK-GROWTH OBSERVATIONS

Although lattice trapping is a predicted result for a cradk in any lattice, the magnitude of the effect depends on the details of the "loadk side" of the force law and on its range. Theoretical estimates do not suggest it should be a ubiquitous and easily observed effect, and, indeed it seems to have been observed unambiguously as a slow crack growth in vacuum only in silicate glasses. Even in these systems, the crack-growth curves are very steep, and thus hard to observe. Such slow crack growth has been looked for in Sä, where the calculations of Sinclair<sup>32</sup> reported above suggest an inbservable activation energy, but so far the material has not been studied iin is sufficiently high vacuum for the result to be conclusive.

When it comes to chemically enhanced fracture, however, thermally activated slow crack growth is very widespread. However, tonly in the brittle systems is there general agreement about the effect of theichemistry. In glasses, where slow crack growth has been most extensively studied, the mesults have been reviewed recently by Wiederhorn *et al.*<sup>76</sup> and Lawn.<sup>77</sup> Briefly, chemically enhanced crack growth in glass is characterized by three regions as shown for H<sub>2</sub>O in Fig. 32. Region I depends on the H<sub>2</sub>O wapor pressure, and the stress intensity factor, as the general reaction-rate theory suggests. At a certain velocity, Region II, the crack outruns the adsorption rate on the crack tip, and the velocity is independent of stress. Then when the crack meaches the intrinsic fracture stress, the velocity curve (Region III) is similar to that in a vacuum. Stage-III fracture still exhibits some atmosphere-dependent effect which is thought to be a dielectric effect on the bonds at the tip by the water.

Michalske and Freiman<sup>78</sup> have proposed that the water reaction features both hydrogen and electron donors in the reaction, leading to enhanced crack growth. Consistent with this proposal, they have also shown that molecules with a similar capability such as  $NH_3$ ,  $N_2H_4$ , and  $CH_3ND$  have similar crack growth curves. The crucial role of hydrogen is confirmed by the fact that  $D_2O$ has a slower growth than  $H_2O$ .

In further work <sup>79</sup> to explore the effect of direct chemical attack at the Si-O bridging bond in simple glasses,  $SiO_2$  doped with network modifiens (Na and Li) have been cracked in a variety of environments. The diffects of the network modifiers have also been studied in molecular-orbital calculations to find the effect of both the bonding and nonbonding Si-O orbital.<sup>80,81</sup> Although the

- <sup>27</sup> B. Lawn, J. Am. Ceram. Soc. 66, 83 (1983).
- 78 T. Michalske and S. Freiman, Nature (London) 295, 511 (1982).





FIG. 32. Slow crack growth of glass in water. Three regions are observed. Region I corresponds to the chemically enhanced growth theory displayed here. In Region II, the external environment is outrun by the crack. Region III is the intrinsic region (after Wiederhorn et al.<sup>74</sup>). (Courtesy of S. Wiederhorn.)

work is still in progress, it appears that the simple ideas expressed in the decomposition theorem above are correct, and can be used to interpret the results.

# VI. Dislocation Emission from Cracks

### 27. INTRODUCTION

According to Part II, one of the two ways to realize a ductile material is if the underlying crack emits dislocations before it cleaves as the external stress is raised. In this section this emission-cleavage dichotomy will be explored.

Historically, this subject was first addressed by Kelly *et al.*,<sup>92</sup> who pointed out that at the tip of a sharp crack, when the K level is high enough to generate cleavage, it is also in the range to initiate spontaneous shear breakdown in the vicinity of the tip. Thus, which event occurs first will depend on the relative

82 A. Kelty, W. Tyson, and A. H. Cottrell, Philos. Mag. 29, 73 (1967).

<sup>&</sup>lt;sup>16</sup> S. Wiederhorn, E. Fuller, and R. Thomson, Metall. Sci. 14, 450 (1980).

<sup>&</sup>lt;sup>19</sup> G. White, D. C. Greenspan and S. Freiman J. Amer. Cer. Spc. 69, 34(11986).

<sup>&</sup>lt;sup>80</sup> B. de Jong and G. Brown, Geochim. Cosmuchim. Acta 44, 451 (1980).

<sup>\*1</sup> B. de Jong and G. Brown, Geochim. Cosmochim. Acta 44, 1627 (1980).
magnitudes of the ultimate strength of the material against tension or/shear. Rice and Thomson<sup>22</sup> analyzed the problem in terms of dislocation emission from the crack tip, because if shear breakdown occurs at the tip, the result is dislocation emission. However, both descriptions are physically equivalent, as has been pointed out by Lin.83 Both of these arguments, however, deal with an essentially atomic property of the tip by quasielastic means, and more exacting attempts have addressed the problem via computer simulation with twodimensional atomic models. However, since only inadequate force laws exist for atoms in the vicinity of such a severe distortion as a crack, these calculations also have major limitations. Thus, the current theoretical situation is not satisfying from a quantitative point of view, though considerable qualitative insight is available. Experimentally, both stable and unstable cracks have been demonstrated, as explained in Part II, and evidence has also been presented there showing that at least under certain conditions dislocation emission and cleavage can coexist in the same material.

In this section, the current status of these effects will be presented. We will begin by reviewing the continuum/cutoff theories, then present the computersimulation results, and close with a discussion of the experimental findings.

## 28. ELASTIC ESTIMATES FOR SHARP CRACKS

Suppose a slit crack in the configuration of Fig. 16 exists, and that no dislocations exist out to a distance large compared with a lattice spacing. Then, a k field can be defined in the vicinity of the crack tip. Assume next!that in the two-dimensional configuration a dislocation is emitted from the crack tip. As a result of the emission (Fig. 33), a ledge is formed at the tip, and an elastic force is exerted between the crack and the emitted dislocation, as calculated in Part IV. For the moment, all effects of any other dislocations in the far field are neglected.

In two dimensions, the total force on the dislocation emerging from the crack is composed of a linear combination of the Mode-I, -II, and -III forces. From Eqs. (15.7), (16.8), and (16.10), the force component in the slip plane is

$$\operatorname{Re}(\overline{f_{d}^{*p}}) = \frac{k_{\mathrm{HI}}b_{*}}{\sqrt{2\pi r}} \cos(\theta/2) + \frac{b_{*}}{2\sqrt{2\pi r}} [k_{1}\sin\theta\cos(\theta/2) + k_{\mathrm{H}}(2\cos(3\theta/2) + \sin\theta\sin(\theta/2))] - \frac{\mu}{4\pi r} \left(b_{*}^{2} + \frac{b_{*}^{2}}{1-\nu}\right). \quad (28.1)$$

The expression breaks down into terms bilinear in b and K (direct k-field force), and other terms quadratic in b (image terms). For a positive b which <sup>33</sup> 1. H. Lin, J. Mater. Sci. Lett. 2, 295 (1983).



blunts the crack, these forces oppose one another, as graphed schematically in Fig. 34. We have used the lower-case k in Eq. (28.1) because it refers to a bare crack without other dislocation effects. According to this result, there is always an attractive force for sufficiently small values of r, and a repulsive force for sufficiently large values of r, because of the different functional dependence on r of the image and k-field forces. Thus, on the basis of purely elastic effects, a crack will always be mechanically stable against the spontaneous emission of a dislocation. But for values of r smaller than the core size of the dislocation and crack, the elastic approximation breaks down. Thus, if the zero in the function of Eq. (28.1) occurs for values  $r_0 > r_c$ , where  $r_c$  is a measure of the effective core size, and  $r_0$  is the radius for which  $\tilde{f}_1^{*p} = 0$ , then emission will occur spontaneously, because by the time a dislocation is "well formed," it already sees a repulsive elastic force, and it never traverses an attractive regime. In other terms, when  $r < r_c$  one might assume the emerging dislocation has a Burgers vector which is proportional to r, and in this regime, the repulsive force becomes dominant until the dislocation is formed. Again, if  $r_0 < r_c$ , then the net force is always repulsive.





If f = 0 in Eq. (28.1), a condition is obtained for  $r_0$  in terms of k, and if  $r_0$  is set equal to the core size  $r_c$ , then, from the discussion above, an equation is obtained for values of k which must be exceeded in order to emit a dislocation.

$$\frac{\mu}{2\sqrt{2\pi}r_{e}}\left(b_{e}^{2}+\frac{b_{e}^{2}}{1-\nu}\right)=k_{\text{HHE}}b_{s}\cos(\theta/2)+\frac{b_{e}}{2}k_{\text{HE}}\sin\theta\cos(\theta/2)$$
$$+\frac{b_{e}}{2}k_{\text{HE}}(2\cos(3\theta/2)+\sin\theta\sin(\theta/2)). \quad (28.2)$$

The added subscript E, on k refers to the critical values for emission.

Equation (28.2) yields a criterion for emission of a dislocation, and the cleavage/emission criterion is obtained by comparing Eq. (28.2) with the Grifflith criterion for cleavage. For simplicity, we first consider the simple case  $k_{\rm H} = k_{\rm HI} = 0$ . Then Eq. (28.2) becomes

$$k_{\rm HE} = \frac{\mu}{\sqrt{2\pi r_e}} \frac{b_e^2 + b_e^2(1-\nu)}{b_e \sin\theta \cos(\theta/2)}.$$
 (28.3)

The Griffith criterion for cleavage is

$$k_{\rm le} = 2\sqrt{\mu\gamma/(1-\gamma)}.$$
 (28.4)

The combined criterion for cleavage/emission in pure Mode I then becomes

$$k_{\rm IE} < k_{\rm Ic}$$
, emission,  
 $k_{\rm IE} > k_{\rm Ic}$ , cleavage. (28.5)

This form of the cleavage-emission criterion was first given by D. Mason.<sup>84</sup>

In their original paper, Rice and Thomson<sup>22</sup> included heuristically in the  $k_{\rm E}$  calculation, a force to produce the ledge. Since the ledge will be fully formed when  $r > r_c$ , any function such as a tan<sup>-1</sup> function which cuts off at  $r_c$  and makes an addition to the surface energy equal to the ledge area will suffice. However, since this term is small compared to the others and is purely heuristic, it will not be included here.

Lin<sup>#3</sup> has shown that the criterion [Eq. (28.5)] for cleavage-emission is physically equivalent to that proposed by Kelly *et al.*<sup>#2</sup> In the latter paper, the cleavate dominance criterion is given as

$$\sigma_{\max}^{\text{tensile}} / \sigma_{\max}^{\text{shear}} > \sigma_{\text{theor}}^{\text{tensile}} / \sigma_{\text{theor}}^{\text{shear}}$$
 (28.6)

 $\sigma_{max}^{\text{tensile}}$  refers to the maximum stress developed in the tensile direction on the atom bonds at the crack tip,  $\sigma_{\text{tensile}}^{\text{tensile}}$  refers to the similar quantity for shear,

$$\mu b/\gamma > 10.$$
 (28.7)

This estimate for cleavage stability can be obtained from Eq. (28.4) by setting  $b_s = 0$ , the angular factors to  $\frac{1}{3}$ , and using  $r_c \sim b_s$ .

Weertman<sup>46</sup> and, much earlier, Armstrong.<sup>87</sup> have also discussed spontaneously generated ductility in the presence of a crack in terms of the stresses necessary to form dislocations outside the crack. Armstrong was led to consider the parameter  $\mu b/\gamma$  in his discussion, and Weertman's results are generally consistent with the criterion Eq. (28.7).

A detailed discussion of the predictions contained in Eqs. (28.3)-(28.5) will be found in Rice and Thomson.<sup>22</sup> Ohr and Chang<sup>88</sup> have applied the same analysis to Mode-III cracks and compared the results with Mode-III thin-foil experiments. (Since the Mode-III experiments involve analysis of dislocation pileups, the full discussion of this paper will be found in Part VII.) The results of these two papers are shown in Table I.

The most clear-cut interpretation of Eq. (28.2) in terms of emission is in terms of a pure Mode-I crack discussed above. However, an important question relates to how a mixed-mode loading might change the results. The first question, however, to be explored is whether the Griffith criterion, Eq. (28.4), is modified by mixed loading. Sinclair and Finnis<sup>89</sup> have indeed suggested without justification that Eq. (28.4) should be replaced by

$$[1 - v/2\mu](k_{ic}^2 + k_{iic}^2) + k_{iiic}^2/2\mu = 2\gamma$$
(28.8)

when all modes of loading are present. (We have added the term in  $k_{\rm HI}$ , which was not in their paper.). Presumably the reason for considering such a generalization of Eq. (28.4) is that (28.8) represents a balance between total elastic force on the left with surface tension on the right, and that  $k_{\rm H}$  and  $k_{\rm HI}$ contribute to the elastic force on an equal footing with  $k_{\rm L}$ .

But Eq. (28.8) is not physically correct, because when  $k_1 = 0$ , no surface is created at all! What is involved is a rather subtle core effect at the crack tip as cleavage takes place under mixed loading. The situation is depicted in Fig. 35.

<sup>&</sup>lt;sup>84</sup> D. D. Mason, Philos. Mag. 39, 455 (1979).

<sup>&</sup>lt;sup>#3</sup> E. Orowan, Rep. Prog. Phys. 12, 185 (1949).

<sup>&</sup>lt;sup>84</sup> H. Weertman, Philos. May. 43, 1103 (1981).

<sup>&</sup>lt;sup>87</sup> R. Armstrong, Mater. Sci. Eng. 1, 251 (1966).

an S. M. Ohr and S. Chang, J. Appl. Phys. 53, 5645 (1982).

<sup>\*\*</sup> J. E. Sinclair and M. W. Finnis, in "Atomistics of Fracture" (R. Latanision and J. Pickens, eds.), p. 1047. Plenum, New York, 1983.



Fig. 35. Mode-II fracture as dislocation formation. In (a) a crack is formed by making abilit in a lattice. In (b), Mode-II forces are applied, and in (c), the bonds are allowed to reweld, because no vertical displacement occurs.

Shown there is a Mode-II crack which moves to the right by one lattice spacing. The result when the bonds facing one another on the cleavage surface are allowed to reweld is a dislocation. If sufficient k, loading is present to separate the crack to the left of the dislocation core region, a crack can result. Since the core region of the dislocation is always of order b, the presence of  $k_{\rm H}$ loading cannot have lowered the critical  $k_1$  needed to hold the cradk open much below its Griffith value, Eq. (28.4). Thus the effect of mixed loading on the Griffith condition is expected to be minor, but to depend quantitatively in a complex way on the details of the atomic bonding in the tip region. For our purposes, it will be sufficient to retain the form of Eq. (28.4) as the cleavage criterion, but remember that the critical  $k_1$  value will depend (only slightly) on  $k_{\rm H}$  and  $k_{\rm H}$ . Of course, if cleavage and emission are closely balanced in Eq. (28.5), mixed-mode loading could affect this balance for emission in Mode I (see Part VII). We note in passing that lattice trapping could be drastically altered by mixed loading, because that is a property also dependent on the details of the atom bonding.

The effect of mixed loading on emission can now be divided into two separate categories. In the first, emission will be considered onto the crack plane itself where  $\theta = 0$  (Fig. 36b,c). Such emission will not blunt the crack. In the second, emission is on a plane inclined at a finite angle to the crack plane, as in Fig. 33.

When emission is on the crack plane, then the elastic forces from  $k_{\rm H}$  and  $k_{\rm H}$  are at their maximum values, while the  $k_{\rm I}$  elastic force is zero. Thus, for a pure edge on this plane, the condition for emission is

$$k_{\rm HE} = \frac{\mu}{\sqrt{8\pi r_{\rm c}}} \frac{b_{\rm c}}{1-\nu} \sim \frac{\mu}{1-\nu} \left(\frac{a_0}{8\pi}\right)^{1/2},$$
 (28.9)



FK3. 36. Emission in Modes I, II, III. In Mode I, the emission force is on an edge on a plane at an angle to the crack, while in Modes II and III the maximum emission force is on the crack plane. A separate requirement is that slip planes exist in these directions.

and for a pure screw,

$$k_{\rm inte} = \mu b_{\rm s} / \sqrt{8\pi r_{\rm c}} \sim \mu \sqrt{a_0} / 8\pi.$$
 (28.10)

In these equations,  $a_0$  is a number approximately equal to a lattice spacing.

These equations describe a condition in which the tensile and shear loadings are independent of one another. Remembering that the role of  $k_1$  is simply to hold the crack open, once that is assured, then emission on the crack plane is simply a matter of building up the  $k_{\rm H}$  or  $k_{\rm H}$  loadings to their critical values.

In the second case, when emission of the dislocation corresponds to the blunting configuration of Fig. 33, then the full generality of (28.2) is required. Now,  $k_{\rm H}$  and  $k_{\rm H}$  loadings either lower or raise the value of  $k_{\rm I}$  required to emit the dislocations depending on the sign of k.  $k_{\rm H}$  loading acts on the screw component, and  $k_{\rm H}$  on the edge. In many cases, simple materials have sufficient symmetry in the cleavage and slip systems available that for a given slip system, such as shown in Fig. 36a, another equivalent slip plane exists mirrored in the cleavage plane. Also, screw components can often be either  $\pm b$ . Hence, mixed loading will in general break the degeneracy in the emission, and favor one system over the others. Quantitatively, the critical value of  $k_{\rm I}$  from Eq. (28.2) becomes

$$k_{\rm HE} = k_{\rm HE}^0 - \frac{2k_{\rm HH}}{\sin\theta} \frac{b_{\rm s}}{b_{\rm e}} - k_{\rm H} \frac{2\cos(3\theta/2) + \sin\theta\sin(\theta/2)}{\sin\theta\cos(\theta/2)}.$$
 (28.11)

 $k_{iE}^{0}$  is the value of  $k_{iE}$  without  $k_{iII}$  and  $k_{II}$ , i.e., given by Eq. (28.4).

Equation (28.11) poses a critical problem to the theory of the cleavageemission balance, because in the simple criterion, Eq. (28.5), both  $k_{le}$  and  $k_{lE}$ are modifed by mixed loadings. We have argued that  $k_{le}$  is not changed in a

	k <sub>ic</sub> Eq. (28.3) Ref. 22	k <sub>ii</sub> Eq. (28.2) Ref. 22	k <sub>ин</sub> Eq. (28.10)	k <sub>ille</sub> IObs. Rzf. 100	E <sub>sct</sub>
Cu	6.4	3.21	1.5	0.4	
Al	3.4	2.17	1.0	0.7	
Ni	8.4	5.47	2.6	1.4	
Fc	8.8	9.34	4.2	1.4	
Mo			8.2	9.2	2.2 (22)
MgO	8.4	29.1	14	Cicaves	
Si	6.4	14.7	8.2	CACRACE	205 (22)*
			0.4		111 (22)
					D.5-1.0 (92)

TABLE 1.  $k_e$ ,  $k_e$ , and  $E_{\rm act}$  for Selected Materials\*

\*k in 10<sup>5</sup> N m<sup>3/2</sup>. E in eV.

\* The numbers in parentheses are references.

major way by addition of  $k_{\rm H}$  or  $k_{\rm H}$ , but Eq. (28.11) suggests that  $k_{\rm H}$  can be. This situation has not been explored sufficiently, experimentally. It may be connected with the appearance of dislocations at cracks in materials supposed to be brittle on the basis of Table I, or vice versa.

## 29. THERMALLY ACTIVATED EMISSION

The previous discussion envisioned a 2D crack and emergent dislocation, which was entirely adequate in discussing the mechanical stability of a sharp crack tip against dislocation emission. But as noted in that analysis, the system always has a lower energy when an emitted dislocation is iar enough from the crack, because the force is repulsive when  $r > r_0$ . In two dimensions, of course, total energies of cracks and dislocations are always infinite because of the infinite length of crack and dislocation. In 3D, however, when the sharp crack is mechanically stable, there will always be a saddle-point configuration of a dislocation loop of finite size through which, in principle, the loaded crack can emit a dislocation by thermal fluctuation. In any discussion of crack stability, the activation barriers for emission by mechanically stable cracks will be an important quantity. It will not be surprising that such a 3D calculation has not yet been carried out in a rigorous way, because of the mathematical difficulty. However, estimates have been formed of the energy barriers.

The first point to note is that in isotropic elasticity, and Mode I, the dislocation loop must meet the crack line at a right angle, because there is no lateral force on the dislocation from the crack, and the dominant force near the tip is the attractive image term. Secondly, the maximum in the function of Eq. (28.2) is a broad one, because of the counteracting effects of the  $1/\sqrt{r} k$ 





Fig. 37. Mode-I emission in 3D. Dislocations must be nucleated from a mechanically stable crack. In (a) the shape of the critical nucleus is assumed to be a half-circle, and in (b) a rectangle.

term and the 1/r image term.<sup>22</sup> Thus, although the stress or force field near the tip is inhomogeneous, there is a large region near its maximum, where the force is nearly constant. For this reason, Rice and Thomson<sup>22</sup> suggested that a likely estimate of the saddle configuration is a half-circle in the classic Frank-Read<sup>90</sup> configuration (Fig. 37). On this basis, the energy of the dislocation loop in Mode I was calculated, using the 2D force expressions, Eq. (28.1). The energy barriers calculated for circular loops in Table I (those from Ref. (22)) are all very large compared with thermal energies in all materials investigated, except iron, which is considered borderline.

Haasen<sup>91</sup> suggested that the earlier values of Rice and Thomson might be too large in the case of Si, because splitting the dislocation lowers its selfenergy, and the stacking fault energy in Si is low. He has estimated about

- \*9 J. Hirth and J. Lothe, "Theory of Dislocations," 2nd Ed. McGraw-Hill, New York, 1982. \*1 P. Haasen, in "Atomistics of Fracture" (R. Latanision and J. Pickens, eds.), p. 707. Plenum,

0.5 eV for the barrier energy of a loop. Lin et al.<sup>92</sup> have also carried out an estimate of the loop energy for Si. In addition to allowing the dislocation to split, they also chose a rectangular configuration "loop" with variable size and aspect ratio. Again, the energy barrier for Si is dramatically lowered over the value of Rice and Thomson, as shown in Table I. The decrease in activation energy calculated by Lin et al. was about equally due to the altered shape of the loop, and to the dislocation splitting.

All these calculations use the 2D force expressions, and are therefore not self-consistent 3D elastic calculations. Because of the relatively large loop sizes estimated in these calculations, the elastic estimate of the energy barrier does not suffer from the atomic cutoff limitation which the 2D stability calculation of Part VI,28 does. Hence, the energy-barrier calculation is apparently one which can be performed legitimately in the elastic approximation. In view of the apparent sensitivity of the estimates to the details of the calculation, a more ambitious rigorous 3D calculation of a suitable crystal is needed. Further, the mixed loading effects discussed in the previous section have not been investigated, and undoubtedly would be of interest as well.

#### **30. ATOMIC CALCULATIONS**

Extensive atomic simulations have been carried out for 2D crackdislocation configurations. Such simulations relate directly to the most crucial issue regarding dislocation emission, namely the crack stability; so they have an important place. Fortunately, as noted in the previous subsection, atomic effects apparently are not germane to the problem of the energy barrier, because 3D simulations are not currently practicable.

We have already dealt in Part V with the general theory of discrete calculations, and report here simply the results. Dislocation effects in simulations were first observed in the work of Wiener and Pear,<sup>93</sup> who found that in the limit of very high driving forces, and velocities, dislocation emission was enhanced by the higher stress required to move the crack at a high velocity. A series of simulations of iron using the Johnson<sup>56</sup> potential were carried out by the Battelle group<sup>58</sup> in various ways, showing that simulated iron was borderline between cleavage and emission. De Cellis *et al.*<sup>60</sup> have simulated iron (i.e., bec metal) with the Johnson potential and copper (i.e., fec metal) with a Morse potential in a calculation with improved treatment of the boundary conditions, and have concluded that these simulated materials have cracks, respectively, stable and unstable against dislocation emission. Multins<sup>41</sup> has performed similar calculations on simulated iron under mixed loading conditions, and finds that the general predictions of the continuum theory is correct. That is, the crack can be made to change its cleavage plane abruptly by addition of Mode II, and the emission criterion is altered by mixed loading. A "phase diagram" from his work, showing how the emission criterion changes under mixed loading, is given in Fig. 38.

All previous calculations have attempted to simulate a particular material by choice of a suitable force law, and they all embed a discrete lattice within a surrounding continuum, with boundary conditions set on the interface between the two regions. In a series of papers, Paskin, Dienes and coworkers<sup>AJ-66</sup> have taken a different approach to the simulation problem. Realizing that no adequate force laws yet exist for real materials, they have carried out a series of molecular-dynamics calculations on a large 2D array with up to 10,000 lattice points using the Lennard–Jones potential. The points in the array form a triangular lattice. The point of view of these investigations is thus to model general fracture phenomena, rather than to make predictions for particular crystals. They have shown that under static conditions, their model will barely support a sharp crack, and that the criterion of Eqs. (28.3)-(28.5) is satisfied. This simulated material thus provides a sensitive test for the validity of the continuum approach, which is encouraging. In their simulations, when the external stress is raised, the crack propagates, and under these





<sup>&</sup>lt;sup>92</sup> I. H. Lin, T-Z Chuang and R. Thomson, to be published (1986).

<sup>&</sup>lt;sup>9.3</sup> T. H. Wiener and M. Pear, J. Appl. Phys. 46, 2398 (1975).



Fig. 39. Results of a computer simulation with small atoms substituted for initial atoms at the surface, as shown by circles. The initial model was ductile. After substitution, dislocation generation is followed by initiation of a new crack (after Paskin *et al.*<sup>44</sup>).

conditions, as in Wiener and Pear,<sup>93</sup> the crack emits dislocations as it cleaves. In the simulations, furthermore, it is observed that virtual emission of dislocations take place. That is to say, when the crack is moving rapidly, an emitted dislocation does not move far after emission, and the dislocation falls back into the cleavage plane after the crack moves on.<sup>63</sup> Such virtual emission was first proposed by Knott<sup>94</sup> in order to explain why the "Griffith. y" for brittle fracture as measured in iron is nearly an order of magnitude higher than the true y is believed to be. If virtual emission occurs during cleavage, it will be an energy-dissipation mechanism, which will add to the measure of  $\gamma$  in the Griffith criterion.

Finally, Paskin et al.<sup>64</sup> have studied the modification of the fracture processes in their model when the atoms in the tip region possess altered bonding properties. Figure 39 shows simulation results when "small" and "large" atoms are substituted at the crack tip, simulating the formation of a surface film at the crack tip. In the one case, dislocation emission is enhanced by the film; in the second, the material is embrittled by the additional stresses induced by the film. In effect, what transpires when a film forms is that the stress singularity at the crack tip is no longer characterized entirely by a local k field, but by the stress field of a precipitate particle. Thus, the discussion of dislocation emission leading up to Eqs. (28.3)–(28.5) no longer applies. The modified analysis using continuum ideas has been carried out by Sieradsky.<sup>93</sup> We will return to additional discussion of the embrittlement question in Part VII.

In a completely different approach, Sinclair<sup>54</sup> has used the lattice-statics discrete-Green's-function approach to study the problem of dislocation emission. Preliminary results only have been reported at the time of printing.

but this powerful approach is being used to explore the effect that force law and crystal symmetry have on the emission criterion to gain some perspective on how these factors affect the emission criterion in a general law.

## 31. EXPERIMENTAL INVESTIGATIONS

The direct and unambiguous experimental demonstration of dislocation emission and the quantitative study of the dislocation phenomena associated with atomically sharp cracks is exceedingly difficult, even with modern techniques. The clearest examples of rigorously brittle cracks have been provided by the observations of B. Hockey<sup>96</sup> in Si, Ge, Al<sub>2</sub>O<sub>3</sub>, and MgO, all relatively brittle materials. The technique used is to indent the surface of a single crystal by a sharp point, and induce local damage. Cracks thus formed then propagate into relatively undamaged portions of the crystal, where they form isolated entities. The tip region is then cut out of the sample and thinned for transmission electron microscopic examination. In the case of Si, when fracture is induced at low temperature, the final crack tip is completely clean (see Fig. 9b), with no dislocations present at all. In some cases (Fig. 9c) after the crack has moved to a certain position, it retreats presumably because of stress relaxation. In these cases, the former cleavage surface is manifested by a network of misfit dislocations because the surfaces have not come back together in perfect registry. At temperatures above that where dislocations are mobile (Fig. 9b) the cracks are found to be associated with dislocation atmospheres. In Hockey's Si observations, detailed slip-plane analysis is lacking, but the observed dislocations may have been emitted after the crack arrested, or they may have been carried along by the crack stress field as the crack grew from the region around the indenter, where intense deformation has occurred.

In other experiments with bulk samples of Si, Champier<sup>97</sup> has analyzed the deformation fields produced by a stationary crack in a technique first used by St. John.<sup>94</sup> In these experiments, analysis of the dislocation loops formed around the crack shows that only a small fraction of the loops are in the blunting configuration depicted in Fig. 36. That is, the majority of loops are on slip planes which are not parallel to the crack line. Although such loops might also have nucleated spontaneously from the crack line, the activated state would have to be a complete circle instead of a half-loop, and it would appear that the barrier would be larger than for the blunting configuration. The most attractive possibility for the origin of the dislocations constituting the

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\*\* C. St. John, Philos. May. 32, 1193 (1975).

<sup>44</sup> J. Knott, Proc. Int. Conf. Fract., 4th 1, 61 (1977).

<sup>\*\*</sup> K. Sieradsky, Acta Metall. 30, 973 (1982).

<sup>\*\*</sup> B. Hockey, unpublished; see also Lawn et al., Ref. 8.

<sup>\*7</sup> G. Champier, to be published (1986).



FIG. 40. Dislocations generated in the vicinity of a crack in MgO. Cracks in MgO appear to generate dislocations from sources close to, but not at, the crack tip. No dislocations are seen which are believed to emanate from the crack itself (after Hockey<sup>94</sup>).

deformation field is thus inhomogeneities in the material whose stress fields are enhanced by proximity to the crack.

In extensive studies of MgO, where deformation accompanies the crack, Hockey<sup>96</sup> has observed many cases where sources of dislocations operate near the crack position (or near a previous crack position), but only a few where the crack itself may have been the source of the dislocation (see Fig. 40).

In summary, for highly brittle materials, the evidence is clear cut that rigorously atomically sharp cracks exist. At elevated temperatures, dislocation emission from these cracks has not been clearly established as yet, although theory suggests that the activation energy may be sufficiently low at least in Si for it to be observed.

In the bcc metals, which are expected to be borderline emitters, the picture is more complex. The most clear-cut experiments have been those of Ohr and co-workers<sup>10,11</sup> using thin film *in situ* electron microscopy, and Vehoff and Rothe,<sup>49</sup> using bulk samples of iron/Si and Ni in hydrogen environments.

The Ohr configuration is shown in Figs. 12 and 13. Cracks are formed when the region near the hole is deformed. Screw dislocations on the slip plane are

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responsible for the "sliding-off" deformation, in the foil, and originate at the crack line which is short compared to the width of the foil. The analysis of the configuration requires consideration of the pile-up of dislocations, which is a subject for Part VII. However, the existence of a local k at the crack tip is all that is required to invoke the emission analysis. Ohr and Chang<sup>88</sup> have in fact used this analysis to generate the numbers in Table I. This case must, however, be a mixed-mode situation, because the crack line and cleavage plane are inclined to the tensile axis at about 45°. For the screw dislocations emitted on the crack-slip plane shown in Fig. 13, the mixed-mode analysis of Part VI,29 shows that only the  $k_{\mu\nu}$  part of the loading is involved in the emission, and the analysis of Ohr and Chang<sup>88</sup> only considers this part. For the reasons stated in Part VI,29, the emission of the screw dislocations does not imply that cleavage cannot occur in Mode I. That is, there is no cleavage-emission competition in the  $k_{\rm m}$  part of the loading, and emission of screw dislocations will simply take place as soon as the critical  $k_{\text{IIIE}}$  value is reached. Any growth of the crack is due to the Mode-I loading, which of course is necessarily present in order to hold the crack open. (See Part VII, 38 for further discussion

In other experiments, <sup>10</sup> when the crack grows into the thicker part of the foil, the fracture mode changes. In Mo, a zigzag configuration develops with the crack propagating in mixed-mode I/II loading on alternating cleavage planes with Mode-II dislocation emission, as shown in Fig. 41. Again, the crack growth shown is, of course, due to the Mode-I loading, and emission occurs when  $k_{\text{BE}}$  is exceeded, as discussed in Part V1,29. With the pileup of Mode-II dislocations observed, however,  $k_{\text{BE}}$  can be achieved again after a dislocation is emitted only after the pileup moves away sufficiently to allow  $k_{\text{n}}$  to rebuild, or the crack may branch to another slip plane (see Fig. 41). Unlike the screw-dislocations, as discussed in Part VII.



Fig. 41. Cracks in molybdenum in the thicker part of the foil configuration of Fig. 13. Figure shows cracks growing in mixed mode and oscillating between equivalent slip planes (after Ohr et al.<sup>10</sup>).

<sup>99</sup> H. Vehoff and W. Rothe, Acta Metall. 31, 1781 (1983).

In Al,<sup>10</sup> a quite different process takes place in the thicker zone. There, an alternating Mode-I cleavage-emission slide-off process occurs. When the Mode-I crack is arrested, emission occurs, to form the classic wedge configuration. Then, as the specimen thins by the continuing general deformation, sudden initiation and propagation of a clean brittle Mode-I crack occurs for a short distance. This Mode-I crack is, of course, not stable in Al, and its appearance as a dynamic event poses a major problem to which we return in Part VII,39.

Experiments on Fe-2.6 at. % Si and Ni single crystals (reviewed by Vehoff and Rothe94) have been performed on macroscopic samples which also throw light on the cleavage-emission tradeoff. In these experiments, the materials can be made to shift from a fully ductile wedge configuration with crack growth by pure dislocation emission and slideoff, to a highly brittle (but not pure) cleavage condition by controlling the temperature or hydrogen pressure on the sample (see Fig. 11). These experiments show that cleavage and emission can coexist, and that the fraction of one versus the other is variable over a wide range. Careful experimental analysis shows that the action of the hydrogen is at the crack tip itself. The authors show that the results are consistent with the occupation of the special site at the tip with a Langmuirtype expression for the occupation probability. The site has a trapping depth of 49 kJ/mol H in iron, which is approximately equal to that for chemisorption on the surface. Because the fraction of cleavage saturates with hydrogen pressure before pure cleavage is attained, these authors believe that their results are to be correlated with the simple coverage of the site at the tip rather than y, because y does not saturate with pressure. They also reconfirm that addition of O2 impedes the hydrogen effects (an old result), and interpret this as being due to the adsorbtion of  $O_2$  on the surface, which denies hydrogen access to the tip.

For us, the important results are that intrinsic cracks in both iron and Ni are ductile at room temperature and above. At low temperature, the iron is brittle, suggesting that iron is indeed borderline, as predicted by the theory, and that the activation energy for emission is low. With the addition of H, the Griffith y is lowered so that emission is less favored. The quantitative results of the experiments are probably interpretable only in terms of a kinetic treatment which predicts how the filling of the sites at the tip, which leads to cleavage, competes with thermally activated emission.

Finally, experiments in ductile materials by Wilsdorf and co-workers, as reviewed by Wilsdorf," have shown that high-purity ductile metals and certain alloys behave almost exactly as predicted. The systems studied were the ductile metals Au, Ag, Cu, and Al, the borderline metal, iron, and the normally brittle Be. All these metals were of high purity, and failure was by fully ductile processes. Under tension, just as the last ligament of a sample is about to pull apart, however, cracks appear in the resultant thin ligament, with the results

shown in Fig. 14. The single-crystal Be samples in these observations are oriented in the easy-glide direction, so that failure is fully ductile. The typical hole-growth process is apparent in the figure, and the only difference between these experiments and hole growth as observed in an engineering material such as in Fig. 6, is that there are no large precipitates for the holes to nucleate on. A new hole is nucleated in these experiments in the dislocation cell walls. After initiation, the crack grows by cleavage (!) to a typical size of the order of a few  $\mu m$ , and then opens in the crystallographic shape shown either by the classic slide-off mechanism, or by the operation of dislocation sources near a tip of the wedge. The major surprise in these experiments is that again, as in the Ohr<sup>100</sup> experiments on Al, a fast-moving cleavage crack has a finite lifetime in a material that in all other ways behaves entirely in a ductile manner.

## VII. Dislocation Shielding and Fracture Toughness

## **32. INTRODUCTION**

With the help of the ideas and the formalism developed in earlier sections, it will finally be possible to confront here on a fundamental level the central problem of fracture: materials toughness.

This problem has had a long history, in its modern dress stretching back to the classic paper by Griffith<sup>47</sup> in 1920 who worked out the basic overall energy balance between the elastic driving forces on a crack, and the resistive forces against crack advance supplied by the material, as discussed in Part IV, 19. In Griffith's work, he identified the resistive forces as the surface tension, y, of the opening cleavage surface at the crack tip, in the soap-film analogy.

But Griffith's relation, Eq. (19.3), had only very limited applicability to extremely brittle materials such as glass, because of the very weak resistive forces which the true surface tension of solids can supply. Ultimately, Orowan<sup>101</sup> and Irwin<sup>102</sup> independently proposed that Griffith's relations could be generalized to tougher materials if the plastic work  $\gamma_p$ , done by the advancing crack, could also be identified as a resistive term leading to a kind of effective surface energy  $\gamma_{eff} = \gamma + \gamma_p$  and incorporated into Eq. (19.3). In cases of small-scale yielding, plastic work done is proportional to the distance moved by the crack, so identifying it as a type of "surface" work is appropriate. With y in Eq. (19.3) replaced by  $\gamma_{eff}$ , it was found that the modified Griffith relation could, indeed, be applied to the fracture of ordinary tough engineering materials, and the modern field of fracture mechanics was founded. Its success

100 S. M. Ohr, to be published (1986).

102 G. A. Irwin, Int. Congr. Appl. Mech., 9th, Univ. Brussels, 8, 245 (1957).

<sup>101</sup> E. Orowan, Trans. Inst. Eng. Shipbuilders, Scotland 89, 165 (1945).

in tough materials is possible because the plastic work done during fracture can be several orders of magnitude greater than the work done in simply opening new surface, and thus the vastly different fracture resistance in materials such as glass and steel can be encompassed.

The term toughness has been used here several times in a descriptive way. Quantitatively, it may best be identified with the resistive force which the material is able to exert against crack advance, and a measure of it would be  $y_{eff}$ . But  $K_c$  and  $J_c$  at the critical crack condition are also often identified with toughness, and a fourth measure, to be discussed in a later subsection, is the "crack-opening displacement" (COD) measured on the crack at a suitable point. Note that these quantities are not dimensionally equivalent to one another, and are defined in different ways. But relations between them can be obtained by theoretical models; so the four quantities do collectively provide a rather loose operational basis for the general concept of material toughness.

Since the pioneering work of Orowan and Irwin, the field of fracture mechanics has progressed by treating fracture as a stress-analysis problem in terms of continuum elasticity and plasticity. The point of view of this article is quite different, however, because, when continuum fracture mechanics is used to address the question of how the forces are transmitted to the crack tip to open the atomic bonds there, a fundamental difficulty is met. This difficulty is expressed in the Rice theorem<sup>32,46</sup> already mentioned in Part IV,18. According to this theorem, in continuum elasticity and plasticity, when a crack advances, the work done by the machines supplying the external stress is absorbed entirely by the plastic processes in the medium, and none is left over for the surface energy of the opening crack. This result depends upon the assumption that the stress at the tip saturates to a finite value, as it must for any realistic plastic yield constitutive law for a material.

At first glance, because of the smallness of the true surface energy y, relative to  $y_{eff}$ , this may not seem like a serious problem. However, the point is that there is in this approach no way to model the opening of the atoms at the crack tip as in Part V. This paradox will be further illuminated from the standpoint of dislocation theory in Part VII,34. It will be shown there that, if the dislocation shielding zone (treated as a continuum) goes right down to the crack tip, that the local k is strictly zero, and the crack is completely shielded. The stress at the tip is then given by the finite dislocation friction stress,  $\sigma_r$ , which is always less than the bond-breaking stress required at the crack tip. This prediction is thus inconsistent with the existence of a cleavage crack at the tip. Hart<sup>103</sup> has found conditions, however, under which a continuum theory can be developed, but, as discussed in Part VII,39, these conditions relate to behavior near the tip.

<sup>10 V</sup> E. Hart, Int. J. Solids Struct. 16, 807 (1980).

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In continuum mechanics, it has been popular to postulate the existence of a "process zone" near the crack tip where the continuum theory breaks down and events transpire which open the crack. It will be our purpose in this section to highlight this zone, and show how the crack-tip stress field interacts with the dislocations to produce the overall fracture. The complete crack and dislocation configuration must be constructed in a self-consistent fashion taking account of the intrinsic structure of cracks in the material on the one hand, and the dislocation mobility and source distribution on the other. Given the known complexity of dislocation behavior in materials, especially in engineering materials, one can begin to appreciate some of the reasons for the complicated fracture behavior in most materials, and engineering materials in particular.

The plan of this section is to (1) discuss the general conditions for crack equilibrium in terms of the three fundamental crack morphologies, (2) present a one-dimensional Mode-III model of dislocation shielding for brittle materials, and materials whose cracks emit dislocations, (3) discuss mixed-mode cracks, (4) discuss moving cracks, and (5) discuss time-dependent mixed cleaving and emitting cracks.

## 33. EQUILIBRIUM CONDITIONS FOR THE THREE PROTOTYPE CRACK CLASSES

The observationally based descriptive discussion of Part II led to a qualitative breakdown of cracks into three distinct morphological classes: the slit crack, the wedge crack, and the externally blunted crack. These different morphological classes also correspond to three different broad mechanisms of fracture corresponding to differing regions on the ductile/brittle spectrum of material response. (The reader should note that the crack classes to be described here are based on different physical mechanisms for fracture, and are, categorically speaking, different from the modes of fracture (Modes I, II, III) which relate to the way in which external loads are applied to a crack.

#### a. Slit or Brittle Cracks

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The slit crack corresponds to a crack which is atomically sharp at its tip, as in Fig. 42, and its most important attribute in comparison with the other two types of cracks is its ability to propagate rapidly. This crack may be a purely brittle crack as envisioned in the mathematical description of Part III, or it may be a crack which has absorbed a finite number of dislocations on its cleavage surfaces so that the crack surface behind the tip has a greater crack opening displacement, as shown in Fig. 42b. In either case, because of the atomically sharp tip, from the elastic point of view, this crack is characterized

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FIG. 42. In (a) an initially sharp slit crack is shown which activates two sources in its neighborhood. When the antishielding dislocations which are attracted to the crack are absorbed by the cleavage surfaces, they create steps which lead to a finite opening of the crack called the COD. The COD is related to the dislocation Burgers vectors absorbed (and to those remaining) by Eq. (33.3). If the source is not precisely lined up with the crack tip, then the tip remains sharp locally.

by a local k field at the tip. The atomic structure at the tip corresponds to the "decohesion" model depicted for the simple cubic lattice in Fig. 3.

It is assumed here that the crack is stable in the lattice in the sense of Part VI, and that the k to which the crack is subjected is less than that at which "decohesion" model depicted for the simple cubic lattice in Fig. 3.

When the criterion for cleavage is met, Eq. (28.5), then the static equilibrium condition for the crack and any associated dislocation cloud (screening and/or antiscreening) is that each defect in the total configuration is subjected to a net zero force. That is to say, the elastic driving forces derived and discussed in Part IV are exactly balanced for each defect by other forces supplied by the material. In the thermodynamic sense, this criterion for the brittle crack is met by the Griffith condition, Eq. (25.3)

$$f_{\rm bc} = 2\gamma. \tag{33.1}$$

In this equation, y is the surface free energy in the Gibbs sense, and will be a function of the chemical activity of any external chemical species.  $f_{ie}$  is given in

terms of the local  $k_1$ , and when mixed loading is applied, we will assume that only Mode I assists the crack growth, although some assistance from Modes II and III is possible, as discussed in Part VI,28.

For the dislocations in the total configuration, in equilibrium, similar conditions must be postulated:

$$(f_4)_j - b_j(\sigma_l)_j = 0.$$
 (33.2)

This equation is expressed for the *j*th dislocation in the cloud in terms of an effective friction stress  $\sigma_i$  at the point *j*. Typically, this stress might correspond to a Peierls "stress," or interaction with impurities or a grain boundary. They should not refer to interactions with other dislocations, except in special cases, because we shall usually include these interactions in the elastic forces explicitly on the left-hand side of Eq. (33.2).

One of the major difficulties met in applying Eq. (33.2) to real situations is that the interactions envisioned in the second term are usually three dimensional in character, while the formalism adopted here is only two dimensional. Thus, some appropriate averaging process to collapse the third dimension is always envisioned, because the enormity of a full threedimensional description is far too great to countenance in its entirety.

The coupled equations (33.1) and (33.2) represent a complete set of conditions for two-dimensional equilibrium. A direct attack can be carried through when the number of dislocations is small or other simplifications are made, but generally speaking, successful attacks on the problem involve rather drastic approximations.

## b. Wedge Cracks and Slide-Off

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The wedge crack in its pure form is one where the crack is unstable against dislocation emission, and its characteristic shape is determined by the geometry and symmetry of the dislocation slip planes at the crack tip. In this case, the crack advance is not by opening of bonds, but by ledge formation as the dislocation is emitted. Thus one dislocation must be emitted for each Burgers vector increment of crack advance. The wedge is formed therefore by alternate "sliding-off" on the equivalent slip planes at the crack tip, as in Fig. 43. This crack morphology was first recognized conceptually by Cottrell<sup>104</sup> and is best confirmed observationally in the work of Vehoff and Rothe,<sup>99</sup> as shown in Fig. 11. Cottrell believed that the slide-off mechanism would not be observed commonly because the crack can only continue to advance without limit if the dislocations continue to advance toward the external surfaces until they exit from the material there. This is exactly what Vehoff and Rothe observe, of course, in their single crystal specimens.

104 A. H. Cottrell, Proc. R. Soc. London Ser. A 285, 10 (1965).



Fig. 43. In an initially sharp slit crack, when  $k_a < k_c$ , as the stress is raised, alternate emission from the tip on equivalent slip planes intersecting the crack create a wedge crack whose opening angle  $\alpha$  is complementary to the angle between the two slip planes. Whether slip occurs on slip planes one or many atom planes separated from one another makes no difference to the final result.

#### c. Externally Blunted Crack

When a crack exists in a material containing bulk sources of dislocations. then as the external stress is raised, these sources may be activated. Figure 42 illustrates what happens to such a crack. In the two-dimensional description, dislocations are always produced from a source in pairs of opposite Burgers vector. By reference to the relevant force expressions in Part IV, it will be found that the dislocation attracted toward the crack is also the antishielding dislocation. In the formalism of Part IV, this corresponds to a negative Burgers vector. On the other hand, the shielding dislocation (positive Burgers vector) of the pair is repelled when the distance to the crack tip is beyond the range of the image force. Generally, then, one will expect that many of the antishielding dislocations will be absorbed in the open (cleavage) surface of the crack. Starting with a slit crack, the result is a crack with a finite opening called the "crack-opening displacement" (COD) given by the total absorbed Burgers vector. Given that the total Burgers vector is conserved during source operation, i.e., by production of compensating pairs, the COD, aside from a cosine factor, is just equal to the remaining total shielding Burgers vector,

$$COD = \sum_{j} h_{j} \cos \theta_{j}.$$
(33.3)

 $\theta_j$  is the angle made between the crack plane and the Burgers vector. Note that the COD by this definition does not include the elastic part of the crack opening which even a slit crack has by virtue of Eqs. (9.13)-(9.15). This



FIG. 44. When a slit crack is blunted continuously by external sources, the crack tip eventually takes on a rounded macroscopic shape because of the randomness of the plastic process. The rounded crack is then best treated from a continuum approximation.

expression is also valid, of course, if the source of dislocations is the crack tip itself.

If the material surrounding a crack is sufficiently soft, then, as the external stress is raised, it may transpire that neither  $k_{IE}$  nor  $k_{ie}$  is ever reached, and continued operation of the external sources progressively blunts the crack, as discussed in Part II. Figure 44 (and Fig. 7) is a schematic drawing of successive blunting and hole formation, in the way presumed to lead to fully ductile fracture. Wilsdorf's observations in Fig. 14 of very clean thin films, although showing highly crystallographic features, is apparently also an example of the same process. Crack advance in the ductile case is possible only because of the nucleation and coalescence of new holes, and the COD is controlled by the distance between the large holes. Otherwise the material will simply neck to rupture on a macroscopic scale, as in Fig. 1.

Analysis of this case is obviously very complicated, and much effort has been expended on it in the continuum mechanics and materials communities. Although this work will not be reviewed here, the major result is that the maximum triaxial stress in front of a blunted crack occurs at a distance in front of the crack roughly equal to the radius of curvature of the tip. When this region of maximum stress reaches out to precipitate particles in the bulk, they fail, and a new hole forms, as shown in the figures of Part II. For a general review of this subject, see Knott,<sup>105</sup> and Rice.<sup>32</sup>

In principle, the processes of ductile fracture have little to do with fracture as we have described it in this article, because only in the early stages of hole formation do any events involving bond breaking occur. However, on a gross

103 J. Knott, Proc. Int. Conf. Fract., 4th 1, 61 (1977).

macroscopic level, the failure is cracklike because the COD is given by the hole size, and this of course is on a scale given by the material microstructure. But even on an atomic scale, the hole-growth mechanism can switch over to cleavage when conditions at the tip change, as for example by chemical embrittlement. Thus the important conclusion is that it is the relative size of  $k_E$ ,  $k_c$ , and  $k_s$  which governs which of the physical classes of fracture occurs. (Here  $k_s$  is a measure of the k necessary to activate sources in the medium in a continuous manner.)

#### d. Mixed Fracture Classes

The previous discussion has arbitrarily separated the three classes for didactic reasons, when the more usual case, and the more interesting one, involves a mixture. Thus, very few materials are so brittle that no dislocations are emitted, or created by external sources. Indeed, one of the major purposes of this article is to consider the shielding provided by such dislocations, and the source of these dislocations must have been either the crack tip or external sources. If the conditions at the crack tip do not turn decisively in only one direction, so that for example alternating emission and cleavage can occur, or alternating cleavage and external source activation, then significant toughness can be generated for a crack which remains atomically sharp (or nearly so) at its tip. It is toward such a crack and the conditions for its existence that the main discussion of this section will be directed.

In the same way, the careful distinction made here between the externally blunted and wedge cracks is also probably not a sharp dividing line in real materials. In the thin-foil experiments of Wilsdorf (Fig. 14), emission and external dislocation generation are observed in the same specimen, Also, the double-wedge configuration taken by the "holes" of Wilsdorf generate longrange stress not unlike that of a smoothly rounded crack, so that hole generation ahead of the crack is to be expected (and is observed!). Thus it is probably moot whether the typical hole-growth mechanism in its later stages as seen in ductile polycrystalline materials is due primarily to dislocations emitted from the crack itself or to external sources.

On the other hand, in the opinion of the author, the crucial question of whether a material will be capable of sustaining a brittle crack stably in a cleavage mode, without blunting the tip and arresting the bond+breaking process, will be determined by the emission of dislocations at the tip rather than by absorption of externally generated dislocations. The reason is that the externally generated dislocations must collide exactly with the tip in order to blunt it, which is an unlikely event, whereas dislocations emitted from the crack blunt the tip by definition. However, the precise conditions under which external sources can halt a cleaving crack are important and unknown at the time of writing.

## 34. ONE-DIMENSIONAL DISLOCATION DISTRIBUTION

If dislocations are distributed along the cleavage plane in front of the crack in a one-dimensional array, the problem of finding the equilibrium distribution is amenable to analytic treatment, if the number of dislocations is large enough to be considered from a continuum approximation. The first such treatment was by Dugdale (Mode 1),<sup>106</sup> followed shortly by Bilby *et al.* (Mode 111),<sup>107</sup> hereafter called simply BCS. In the BCS theory, the crack is considered to be a continuum distribution of virtual screw dislocations whose Burgers vector distribution,  $\beta(x)$ , is related to the crack displacement  $u_3$  by the equation

$$u_3 = \frac{\partial \beta}{\partial x_1}, \qquad db = \beta(x_1) dx_1. \tag{34.1}$$

(See Part II,4.) These virtual or "crack" dislocations are set in equilibrium with each other and with the external stress distribution at the point x on the cleavage plane. The resultant distribution thus gives zero stress on the cleavage plane, and therefore "solves" the crack problem. The stress external to the crack is then just that provided by the "crack" dislocations, and the results are equivalent to that of Part III. BCS, however, go further and let a distribution of "real" dislocations be placed on the external cleavage plane, and then solve the total equilibrium problem of "crack" plus "real" dislocations. The external dislocation distribution is presumed to start at the crack tip. The BCS theory has been used extensively to interpret the plastic zone of cracks, because its results are analytic and easy to understand.<sup>108</sup> The BCS theory is a direct extension of dislocation pileup theory to a situation where the stresses are inhomogeneous, and, because of this simple picture, the BCS description has thus been very appealing to those familiar with dislocation theory.

An extension of the BCS model was developed by Chang and Ohr<sup>58,109,110</sup> to explain the experimental results by Ohr and co-workers<sup>10,111-117</sup> and

100 D. S. Dugdale, J. Mech. Phys. Solids 8, 100 (1960).

107 B. A. Bilby, A. H. Cottrell, and K. H. Swindon, Proc. R. Soc. London Ser. A 272, 304 (1963).

140 E. Smith, in "Dislocations in Solids" (F. R. N. Nabarro, ed.), Vol. 5, p. 364. North Holland Publ., Amsterdam, 1979.

109 S. Chang and S. M. Ohr, J. Appl. Phys. 52, 7174 (1981).

110 S. Chang and S. M. Ohr, Int. J. Fract. 23, R3 (1983).

111 J. Narayan and S. M. Ohr, Proc. Int. Conf. Electron Microsco, 9th 1, 580 (1978).

112 S. Kobayashi and S. M. Ohr, Proc. Annu. Meet. EMSA, 37th p. 424 (1979).

113 S. M. Ohr and J. Narayan, Philos. Mag. A41, 81 (1980).

114 S. Kobayashi and S. M. Ohr, Philos. Mag. A42, 763 (1980).

115 S. M. Ohr and S. Kobayashi, J. Metall. 32, 35 (1980).

110 S. Kobayashi and S. M. Ohr, Scripta Metall. 15, 343 (1981).

117 J. Horton and S. M. Ohr, J. Mater. Sci. 17, 3140 (1982).



Fig. 45. Dislocation shielding configurations. (a) A Mode-III slit crack is depicted with a distribution of screw dislocations on its cleavage plane. The solid curve represents a continuous distribution function of the same set of dislocations, on the interval from  $x_1 = c$  to  $x_1 = d$ .

Chia and Burns<sup>118</sup> on dislocations emitted from cracks which showed a dislocation-free zone near the crack tip. The path to be followed here is a further simplification of their work, published independently by Majumdar and Burns<sup>119</sup> and by Weertman *et al.*<sup>120</sup> Starting with BCS, all the mathematical developments make essential use of the Muskhelishvili integral equation of the Appendix.

In the following, the description will be a Mode-III crack in antiplane strain, but the analysis is also applicable to Mode I with edge dislocations with Burgers vectors perpendicular to the cleavage plane or Mode II with Burgers vector in the cleavage plane. To make the transition from Mode III to Mode I or II, simply make the substitution  $\mu \rightarrow (1 - \nu)\mu$  in the equations. In Mode III and II, the cleavage plane is a glide plane, while in Mode I, the dislocation motion in the cleavage plane is by climb.

Consider a semi-infinite Mode-III crack with its tip at the origin, and a distribution of screw dislocations on the  $x_1$  axis as shown in Fig. 45. For such a distribution on the  $x_1$  axis, Eq. (15.7) becomes

$$f_{d} = \frac{K_{\rm m}b}{\sqrt{2\pi x}} - \frac{\mu b^{2}}{4\pi x} + \sum_{j}' \frac{\mu b b'}{2\pi} \frac{1}{x - x_{j}} \left(\frac{x_{j}}{x}\right)^{1/2}.$$
 (34.2)

The subscript on x has been dropped here and subsequently where the meaning is clear.

Making the continuum approximation.

 $db = \beta(x) \, dx.$ 

(34.3)

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Then

$$df_{d} = \frac{K_{\rm m}\beta\,dx}{\sqrt{2\pi x}} - \frac{\mu(\beta\,dx)^2}{4\pi x} + dx \int_{c}^{d} \frac{\mu\beta(x')\beta(x)}{2\pi(x-x')} \left(\frac{x'}{x}\right)^{1/2} dx'.$$
(34.4)

118 K. Y. Chia and S. J. Burns, Scripta Metall. 18, 467 (1984).

119 B. Majundar and S. Burns, Int. J. Fract. Mech. 21, 229 (1983).

120 J. Weertman, I. H. Lin, and R. Thomson, Acta Metall. 31, 473 (1983).

If the distribution is in equilibrium, then from Eq. (33.2)

$$\frac{df_d}{dx} = +\beta(x)\sigma_t(x), \qquad (34.5)$$

and the equilibrium equation (34.5) can be written

$$\frac{2\pi}{\mu}\left(-\sqrt{x}\sigma_{\rm f}(x)+\frac{K_{\rm m}}{\sqrt{2\pi}}\right)=-\int_0^d\frac{\sqrt{x'}\beta(x')}{x-x'}dx'.$$
(34.6)

The term in  $(\beta^2 dx^2)$  is of course dropped because it is a higher-order differential.

Equation (34.6) has the canonical form of the Muskhelishvili integral equation, (A.44), and its solution is given by (A.45).

$$\beta(x) = \frac{2}{\pi \mu} \left( \frac{(x-c)(d-x)}{x} \right)^{1/2} \int_{c}^{d} \frac{g(x')dx'}{(x'-x)\sqrt{(x'-c)(d-x')}},$$

$$g(x') = -\sqrt{x}\sigma_{f}(x) + K_{W}/\sqrt{2\pi}.$$
(34.7)

Because  $\beta$  is assumed to be zero at infinity, all polynomials in (A.45) are zero. If  $\sigma_f(x)$  is a constant, the solution of this equation can be written in terms of elliptic integrals <sup>109</sup> (Fig. 45). The general form of  $\beta$ , however, is seen from the square-root factor in front of the integral in Eq. (34.7). There is thus a sharp maximum near the front edge at c, and a decrease to zero at point d. A solution can also be given numerically<sup>121</sup> for an arbitrary function  $\sigma_f(x)$ .

The continuum solution is only useful when  $c \ll d$ , and for this case when  $\sigma_r$  is a constant, a very simple set of relations can be written<sup>120</sup>

$$k = \frac{3}{\pi} \left(\frac{2}{\pi}\right)^{1/2} \sigma_{\rm f} \sqrt{c} \left( \ln \frac{4d}{c} + \frac{4}{3} \right), \tag{34.8}$$

$$K = 2 \left(\frac{2}{\pi}\right)^{1/2} \sigma_{\rm r} \sqrt{d}, \qquad (34.9)$$

$$\beta = \int_{\pi}^{d} \beta(x) \, dx = \frac{K}{\mu} \left(\frac{2d}{\pi}\right)^{1/2}.$$
 (34.10)

Strictly speaking, in these equations, in Mode III,  $\sigma_r$  must correspond to a friction force on the dislocations, which in the simplest terms would be the Peierls force of the lattice against the dislocations. More generally, though, it could be any other resistive force in the lattice, such as interactions with impurities, or grain boundaries. Such resistance terms are usually thermally

121 N. Loual, unpublished results.

dependent, however, and are not entirely consistent with the time-independent model assumed here.

In Mode I, the stress is usually interpreted as the yield stress, and the reason for this is best seen from Dugdale's original figure (Fig. 46). In a thin plate with a crack under tensile load, the deformation zone is concentrated ahead of the crack because of the tendency of the plate to thin down in this region. The overall effect is that of a distribution of edge dislocations running parallel to the crack tip, and with Burgers vector perpendicular to the crack plane. The opening of the crack, COD, is given by the relation, Eq. (33.3). Since the dislocations are produced by localized yielding in the deformed region, the stress in this region is given by the yield stress  $\sigma_1$ . Without work hardening,  $\sigma_2$ is a constant. Thus, depending upon the details of the modeling, or in Eas. (34.8)-(34.10) and the equations leading to it, may variously take on the meaning of a static yield stress, or a friction force. If the dislocations are thought of as being created by sources in the region of a static crack, then their local density will be fixed self-consistently by that value of or which gives a local stress equal to the yield stress. If, on the other hand, the dislocations have been created, for example out of the crack tip in Mode III, or Mode II, and are mobile, they will move into a configuration consistent with the local frictional resistance forces. These two cases will be discussed in detail in Part VII,35.

When  $c \to 0$  in Eqs. (34.6)-(34.10), the BCS or Dugdale limit is obtained. In that case  $\beta$  is given by an analytic function,<sup>122</sup> and for a finite crack with tips at  $x = \pm a$ ,  $\beta$  is

$$\beta = \frac{2\sigma_{t}\alpha}{\pi\mu} \ln \left| \frac{x\sqrt{d^{2} - a^{2}} + a\sqrt{d^{2} - x^{2}}}{x\sqrt{d^{2} - a^{2}} - a\sqrt{d^{2} - x^{2}}} \right|.$$

$$\alpha = \begin{cases} 1, & \text{screw} \\ (1 - \nu), & \text{edge.} \end{cases}$$
(34.11)

This distribution contains a singularity at the crack tips,  $x = \pm a$ . Equations (34.9) and (34.10) are still valid.

Dai and  $Li^{123}$  have carried out numerical calculations for the equilibrium of a discrete set of dislocations, with Eq. (34.2) directly, with much the same results as shown for the continuum analysis.

The most important result in the BCS limit, however, is that the loca. k disappears, and the crack is completely shielded from the external stress. This result was already anticipated in Part VII,32 in the introductory comments. The point of view expressed in this article is that without a local k at the core crack, the stress environment there cannot be adjusted to the requirements of



FIG. 46. Dugdale configuration. If a thin plate containing a crack is pulled in tension, the plate will slip ahead of the crack on planes through the thickness as shown, leaving edge dislocations running on the inclined planes through the specimen. The two dislocations, however, have the overall effect of a single edge dislocation with Burgers vector normal to the cleavage plane.

local equilibrium for the core crack. That is, if the crack is a cleavage crack, the local k must reflect the requirements of the bond strengths of the atoms at the tip  $(k_c)$ , and if it is an emitting crack, the local k must do the same for emission. On the other hand, if the crack is completely shielded, the stress at the tip is given by the limiting value of  $\sigma_r$ , which is a parameter describing some kind of plastic response of the material, such as the yield stress, and does not provide a value of the ultimate bond strength. Thus a completely shielded crack is an inconsistent solution of the total problem. Nevertheless, Eqs. (34.9) and (34.10) do not contain the crack-tip parameters c and k, and are predicted correctly by the BCS continuum solution. These results are useful by themselves, and indeed, books on fracture such as the classic one by K nott, <sup>124</sup> and the reviews such as the excellent recent one by Smith, <sup>108</sup> make much worthwhile use of the BCS theory and these last two relations.

## 35. THE FRACTURE CRITERION IN CLEAVAGE

As promised in the introductory subsection, Eqs. (34.8)-(34.10) provide a rudimentary form of a fracture criterion. A fracture criterion should predict  $K_e$ 

<sup>122</sup> J. Weeriman, Int. J. Fract. Mech. 2, 460 (1966).

<sup>123</sup> S. H. Dai and J. C. M. Li, Scripta Metall. 16, 183 (1982).

<sup>&</sup>lt;sup>124</sup> J. Knott, "Fundamentals of Fracture Mechanics." Butterworths, London, 1973.

in terms of intrinsic materials variables for crack equilibrium. If  $d_r$  is a true friction stress, and independent of the properties of the dislocation shield, then Eq. (34.8) is decoupled from the other two in the sense that then the first equation relates only to the crack tip region. The weak dependence on *d* in the logarithm can be safely ignored in first approximation. In effect, Eq. (34.8) sets *c* and *k* so they are consistent with one another, independent of the magnitude or extent of the shielding zone. In a sense, there is no predicted  $K_e$ , because it depends on *B* or *d*, which can be set at will. Then, Eqs. (34.8)–(34.10) are underdetermined until some additional information is provided, such as a law giving the magnitude of the shielding charge *B*.

One way to provide the missing information is to identify  $\sigma_t$  as a yield stress, and link it to the local dislocation distribution  $\beta$  by a work hardening law. Such a law, however, would change the character of the integral equation, (34.6), and the solution, Eqs. (34.8)-(34.10) would not be valid. Weertman et al.<sup>120</sup> have proposed that another, less satisfactory constitutive law can be obtained by linking  $\sigma_t$  to the total  $\beta$  by an equation such as

$$\sigma_{\rm f} = \sigma_0 (B/B_0)^{\rm m}. \tag{35.1}$$

With this equation, the set of equations (34.8)-(34.10) is fully determined, and the critical k is given as <sup>120</sup>

$$K = \kappa (k_c^2/c)^{(1+m)/4m}, \qquad \sqrt{2B_0\mu}$$

$$\kappa = \left(\frac{\pi^3}{18}\right)^{(1+m)/4m} \frac{\sqrt{2B_0\mu}}{\sigma^{1/2m} \left(\ln\frac{4d}{c} + \frac{4}{3}\right)^{(1+m)/2m}}, \qquad | (35.2)$$

$$k_c^2 = 4\mu y.$$

In this equation,  $\kappa$  depends primarily on macroscopic quantities, while k and c are tip region parameters.  $k_e$  is the critical k for crack advance, and is given here in terms of the Griffith relation and y. In this form, one sees that, in spite of the large shielding which might be provided by B, the entire fracture process is very sensitively controlled by the conditions of atomic bonding at the tip because of the overall balance and equilibrium which is required. The appearance of c in this relation is interesting. In Eqs. (34.8)–(34.10)  $\sigma_f$  has been identified as a yield stress, but the model does not let local sources of dislocations operate within the elastic enclave x < c, and the physical reason for this is that in real solids, the sources for dislocations are not ubiquitous on an atomic scale. In this picture, then, c is the distance to the first source of dislocations, a parameter which is linked back to the inhomogeneity or graininess of the scale of plasticity in a real material. Without this plastic "grain size," of course, the crack would be fully shielded again, and all the edjections already voiced about that situation would pertain.

Equation (35.2) shows qualitatively the required dependence on the physical parameters  $\mu$ ,  $\sigma_0$  (which is the initial yield stress), work hardening parameter, etc. However, it is based on a very primitive one-dimensional model. Another indiation which uses the inner cutoff idea, but uses a two-dimensional treatment off the plastic region gives a somewhat different and probably better indiation<sup>(23)</sup>

$$K_{c}^{2} = 2\pi \left(\frac{2\gamma\mu}{\pi}\right)^{(1+m)/2m} / (\sigma_{0}^{2}c)^{(1-m)/2m}.$$
 (35.3)

lingthis equation, the work hardening law is written

$$\sigma_{\rm f} = \sigma_0 (\epsilon/\epsilon_0)^{\rm m} \tag{35.4}$$

in the traditional manner, where  $\epsilon$  is the strain, and  $\sigma_r$  is a local function of strain, in which the local strain is related to  $\beta$ .<sup>126</sup> Equation (35.3) is a correction of the original expression in Thomson.<sup>126</sup> Equation (35.3) has been tested against steels which have been embrittled with results which are satisfactory, but no iintensive effort has been made to validate the prediction. The reader will find additional discussion of the elastic-plastic enclave approach by Weertman<sup>127,128</sup> and Fuller and Thomson.<sup>125</sup>

## 1361 EMESSION-CONTROLLED SHIELDING

When  $k = k_e$  dislocation emission occurs. This class of fracture has been istudied intensively in Mode III by S. M. Ohr and his collaborators at Oak [Ridge,<sup>[10,1]1-137</sup> by Wilsdorf and collaborators at the University of Virginia,<sup>6</sup> (by P. |Neumann and collaborators at Dusseldorff,<sup>9,99</sup> and by Chia and Burns.<sup>118</sup>In a typical experiment, as performed by Ohr, a small rectangular specimen is thinned through its center, as shown in Fig. 12. When stressed in the transmission electron microscope, shear is induced in the thin portion of the foil, ias shown in Fig. 13b. If dislocations are injected into the thicker part toff the Koil from the thin edge, eventually when the total Burgers vector component normal to the foil nearly equals the thickness of the foil, the foil shears: apart, and a Mode-III cracklike artifact is formed. From the geometry, in pure ishear, the "crack" line would have zero length at its tip, but in the experiments, some Mode I develops because the crack possesses a small finite length altits tip associated with the dislocation free zone. Figure 13 has already klisplayed results for copper.

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<sup>123</sup> E. Fuller, and R. Thomson, AIME Symp. Micro Macro Mech. Crack Growth 49 (1981).

<sup>196</sup> R. Thomson, J. Mater. Sci. 13, 128 (1978).

<sup>117. 9.</sup> Weurtman, Acta Metall. 26, 1731 (1978).

<sup>&</sup>lt;sup>[1:00]</sup> J. Weettman, J. Mater. Sci. 15, 1306 (1980).

The primary results of these experiments are: (1) the dislocations are emitted on the crack plane (which coincides with a slip plane) from the crack tip as it grows into the foil; (2) there is a significant zone in front of the crack devoid of dislocations, called a dislocation free zone; (3) the number of dislocations emitted is correlated with the thickness of the foil; i.e.,  $COD \simeq \sum b_i \cos \theta_i$ , where  $\theta_i$  is the inclination angle of the slip plane to the normal of the foil; (4) the distance to the first dislocation is a function of the stress on the crack, such that when the stress is lowered, this distance also decreases; (5) the distribution observed is that of an inverse pileup, with a sharp maximum in the vicinity of the first dislocation; (6) when the crack grows into a relatively thick portion of the foil, it often develops more Mode-I character, so that emission is then observed on slip planes intersecting the crack plane at a finite angle, blunting the crack as discussed in Part VI; and (7) quantitative interpretation of the results can be correlated with the emission criteria of Part VI and the shielding results of Part VII,34, to which we now turn.

Chang and Ohr<sup>109</sup> and Ohr and Chang<sup>88</sup> have interpreted these results in terms of the one-dimensional continuum model of Part VII,34 with a finite value of c in Eqs. (34.8)-(34.10). In the experiments,  $\sigma_t$  and c can be measured. From Eq. (34.8)  $k_{\rm HI}$  and  $K_{\rm HI}$  can be calculated. In this case, of course, the critical value of  $k_{\rm HI}$  in Eq. (34.8) is the critical value for dislocation emission, called in Part VI,  $k_{\rm HIe}$ . The results taken from Ohr and Chang<sup>88</sup> are shown in Table I.

Several comments are in order regarding the validity of the models. First, the experiments are performed in thin foils, and the theory pertains to thick specimens. In the elastic analysis, the stresses on the foil faces must be zero [Eq. (7.3)]. If the crack were normal to the foil surface, and the stress state were Mode I or Mode II, then plane stress (see Part III,9) would apply. However, the crack is primarily a shear crack in Mode III, and the axis of the crack and its associated dislocations is inclined to the plane of the foil at a finite angle. Eshelby and Stroh<sup>129</sup> have analyzed the problem of screw dislocations normal to a surface and shown that screw dislocations in that case have a truncated long-range stress field of the form  $r^{-1/2}e^{-r/t}$  (incorrectly quoted in their paper), where t is the foil thickness, because of the image terms in the foil surface. Edge dislocations retain their long-range 1/r stress fields, however. For the same reason which leads to the truncated screw stress field, the Mode-III crack if normal to the foil surface would also be expected to have a truncated long-range stress field in a foil. However, the crack and slip plane are at an inclined angle to the foil, so only a portion of the  $\sigma_{zo}$  and  $\sigma_{zr}$  stress fields will be cancelled by the boundary condition on the foil surface. Thus the inclined crack and dislocation distribution will retain a portion of their long-



FIG. 47. View of fracture plane for the foil. The crack line is a small fraction of the foil thickness, and the thickness is a function of position in the plastic zone. The stress state at the crack line must possess at least a small amount of Mode I in order to open the crack at that point, but the stress cannot be two dimensional because of the variable thickness of the crack plane.

range interactions and the crack and dislocations will interact with one another at distances well beyond the foil-thickness distance. However, buckling in the foil will still serve to orient the system so that the image terms can operate to some extent, and will tend to decrease the long-range interactions further. Chang and Ohr<sup>130</sup> have studied the effect of finite thickness on the integral equation Eq. (34.6) in Mode III, but because of the inclination of the slip plane to the foil surface, the configuration is not pure Mode III as explained above.

The second point concerns the question of whether the geometry of the sheared foil really represents a two-dimensional Mode-III crack. A view of the crack plane would schematically be that shown in Fig. 47. Because of the variable thickness of the foil in the plastic zone, the stress state cannot be entirely two dimensional. In effect, there must be a higher effective k at the crack tip relative to the two-dimensional k used in the equations, roughly in proportion to the ratio of the crack-line length to the undeformed foil thickness. Thus, the foil geometry generates an inherent uncertainty in the two-dimensional antiplane-strain analysis. However, there is no question that the qualitative picture is correct and the surprising quantitative results shown in Table I indicate that the approximations in the analysis are not serious or that they cancel one another.

It is important to note that these Mode-III experiments do not bear directly on the Mode-I emission-cleavage dichotomy of Part VI. The discussion there emphasized the independence of the modes relative to this question, and emission of screw dislocations in Mode III was shown to be unaffected by cleavage events in Mode I. There is an observable short Mode-I crack in the experiments, as shown in Fig. 47, which coexists with the Mode-III emission, but the value of  $k_1$  at the tip has not been calculated. (For self-consistency, of course, it must be at the Griffith value.) The general configuration of the

130 S. Chang and S. M. Ohr, Int. J. Fract. 21, 3 (1983).

<sup>129</sup> J. D. Eshelby and A. N. Siroh, Philos. Mag. 42, 1401 (1951).

overall loading in the (non-2D) foil dictates that the  $k_1$  and  $k_{111}$  values must be about equal, but the detailed analysis has not been carried out. Hence, a direct quantitative comparison of  $k_{111E}$  with  $k_{1E}$  based on these experiments cannot be made. It is very interesting, however, to note that in the same configuration, MgO does not emit screw dislocations, but cleaves, showing that the experiments do have a qualitative bearing on the cleavage/emission dichotomy. These mixed mode loading questions are further pursued in Part VII,37.

The Mode-III foil experiments do not relate directly to any perceived macroscopic failure mode in a bulk material, but they throw a very strong experimental light on two general principles in fracture: They confirm direct emission of dislocations from a sharp crack tip in fcc and bcc metals, and they confirm the general proposition of crack tip shielding including the importance of the local k at the crack tip. However, we suggest there is one important mechanism operating in the failure of practical ductile materials where the Mode-III (or its sister Mode-II) crack discussed here could play a role, and that is the observed shear breakdown found to occur between neighboring holes in the later stages of hole growth fracture. (See Fig. 14.)

Experiments reported by Chia and Burns<sup>118</sup> on cracks in LiF do provide general confirmation of the picture presented here in bulk specimens. An additional feature found, however, relates to the effects of nonblunting glide dislocations in shielding the crack. Unloading in their case also had the interesting effect of increasing the deformation zone in a nonlinear fashion, a result of interest for fatigue crack growth.

The experiments of Wilsdorf and collaborators<sup>6</sup> have focussed on the final stage of ductile rupture of a specimen. Some experiments have been performed on macroscopic sized specimens, which neck to a fine chisel edge, as shown in Fig. 5. TEM studies of the thinned neck during final rupture are similar to results of prethinned foil specimens stressed in situ in the microscope. Figure 14 shows that, just before final rupture, a ductile "crack" develops composed of a regular series of rectangular holes. The nucleation and growth of these holes has been studied in a variety of ductile materials: Ag, Al, Au, Cu, and Fe and Be in the pure form and stainless steel and Al alloys. Both polycrystalline and single crystals were included. For a general review of the results, see Wilsdorf.<sup>6</sup> The major results were: (1) the voids are nucleated in dislocation cell boundaries; (2) the holes formed take a highly crystallographic shape determined by the operation of dislocation sources either at the sharp corners or from bulk sources very near these corners where stress concentrations are high; the void in other words grows at each of its corners by the slideoff mechanism for an emitting crack; and (3) there is an observable difference when the strain rate is "high" typical of that to be expected in a specimen deformed in an Instron machine, and "low" corresponding to a creep regime. In the "high"-strain range nucleation and growth take place by both

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dislocation avalanches and twinning, with resultant regular hole formation. At lower strain rates, individual dislocation events are observable, but the overall results are less regular in appearance, corresponding to the ability of the dislocations to achieve lower-energy configurations by strain annealing. The first stage of hole initiations is the growth of a rapid dynamic brittle crack to a length equal to the length of the final void, and then it stops. Blunting then takes place slowly by deformation at the crack tip. The initial fast dynamic growth is not consistent with the subsequent behavior as a ductile process. In Fig. 48, a high magnification micrograph shows the initiation of a hole in a cell boundary.

Analytic treatment of the emitting cracks of Vehoff *et al.* (Fig. 11) and the growing voids of Wilsdorf and co-workers involves the application of the wedge-dislocation interaction analysis of Part III, and has not been carried very far as yet. The reader is referred to the paper of Chang *et al.*<sup>23</sup>

#### 37. SHIELDING BY EXTERNALLY PRODUCED DISLOCATIONS

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Even for a stable cleavage crack which does not emit dislocations, external sources for dislocations nearly always exist in a material, and when sufficiently close to the crack, the stress concentration can cause them to operate. Lin and Thomson<sup>131</sup> have investigated the shielding provided by a single external source (Fig. 49) and analyzed the stress on the source and the shielding of the crack tip as a function of the number of dislocations produced. Neglecting the effect of ledge formation by the antishielding dislocations which might be absorbed by the crack, they show that the back stress of the dislocations on the source is stronger than the shielding of the crack tip, because the source is closer to the dislocation pileup than the crack is. Thus, as the external stress of the K field is increased, the cleavage criterion at the crack tip will ultimately be achieved again for a finite number of dislocations produced by the source. Thus, neglecting the effect of crack shape change due to dislocation absorption, the crack will remain brittle in the sense that the sources will provide only a limited and finite shielding for the crack. Brittle crack propagation will then always be possible for some value of external K, which depends upon the source location and source hardening parameters.

This model has not been adequately pursued to explore the toughening properties of a discrete distribution of external sources for dislocations. Crossover to the ductile fracture mechanism is inherent in such a model, however, if the shape change in the crack can permanently lower the local kbelow  $k_{\rm H}$  while external sources continue to operate. This question is closely

131 L.H. Lin and R. Thomson, Scripta Metall. 17, 1301 (1983).



FIG. 48. Initiation of a hole near a crack in the Wilsdorf configuration.\* (Courtesy H. G. F. Wilsdorf.)



Fig. 49. Operation of a Frank-Read source near a crack tip.  $\zeta_{PB}$  is the distance to the source and  $\zeta$  to the dislocation loop tip.

related to the phenomenon of blunting the tip by external sources already discussed in Part VII,33. It is important to find out by further theoretical modeling as well as by experimental investigation if external sources can by themselves provide a path for the cleavage-ductile transition in a material without invoking dislocation emission from the crack tip.

Dislocation shielding of cracks in any real case is probably due to a mixture of external sources as well as emission. For example, any emitted dislocation pileups will certainly interact with sources in the medium, and the overall shielding will be a mixture of the two types. Modeling of such situations probably is best accomplished by material-deformation constitutive laws, which suggests that an ultimate "solution" of the practical problem will probably involve a continuum solution of the outer parts of the deformation field with a discrete approach to the inner region reminescent of the lattice modeling of Part V.

## 38. MODE-I AND MIXED-MODE PROBLEMS

The shielding problem in Mode I is sufficiently difficult that relatively little analysis has been carried out for it except for numerical calculations in the 1D BCS approximation. We have given the general 2D results for interactions between cracks and dislocations in Part IV, however, and some general comments can be made here regarding the character of these interactions. The shielding relation, Eq. (16.7), can be written for the real and imaginary components for the contribution  $K_d$  of each dislocation to K as

$$(K_d)_1 = \frac{\mu}{(1-\nu)\sqrt{2\pi r}} \left[ b_2 \cos\frac{\theta}{2} + \frac{\sin\theta}{2} \left( b_1 \cos\frac{3\theta}{2} + b_2 \sin\frac{3\theta}{2} \right) \right],$$
  

$$(K_d)_{\rm H} = \frac{\mu}{(1-\nu)\sqrt{2\pi r}} \left[ b_1 \cos\frac{\theta}{2} + \frac{\sin\theta}{2} \left( b_2 \cos\frac{3\theta}{2} - b_1 \sin\frac{3\theta}{2} \right) \right].$$
(38.1)

The overall shielding situation is somewhat complex, because, not only is there an angular dependence in (Eq. 38.1) which changes sign with  $\theta$ , but for any given crack, there can be a mixed-mode loading. By a mixed mode, we mean that the external loading of the crack can be a combination of Modes I, II, and III. The loading in turn will in general produce the dislocation distributions typical for such loading through dislocation emission.

The characteristic dislocation distributions (from emission events at the crack) will be those depicted in Fig. 50. Figure 51a shows the shielding of a



FIG. 50. Typical dislocation configurations for pure loading situations. Mode 1 produces shielding dislocations on slip planes at an angle to the crack plane.  $(b_x)_1 = -(b_x)_2; (b_y)_1 = (b_y)_2$ . In Mode 11, the dislocations are produced on the plane of the crack, but some cross slip can be expected. In Mode 111, no specific slip plane is necessary because of the screw character of the dislocations, but in practice, the dislocations will tend to be formed on the crack plane. In each mode, as the crack moves forward, the dislocations will be left behind as a wake. 109



FIG. 51. In (a), the  $K_d$  shielding contribution to Mode I of a dislocation with Burgers vector  $(1/\sqrt{2}, 1/\sqrt{2}, 0)b$  is displayed as a function of angle  $\theta$  relative to the crack tip. See Eq. (38.1). In (b) angle to the crack tip.

dislocation with Burgers vector  $b = b (1/\sqrt{2}, 1/\sqrt{2}, 0)$  as a function of angle relative to the tip. Maximum shielding occurs roughly at the  $\theta \simeq \pi/2$  point. Dislocations on the two slip planes shown in Fig. 50a contribute symmetrically to  $K_1$ .

When a Mode-II dislocation interacts with a Mode-I crack, cross slip is assumed to spread the dislocations off their initial slip plane, which is coincident with the crack plane, into a thin region on either side of the crack plane in a symmetrical manner (Fig. 50b). The second term in the first equation of Eq. (38.1) is the relevant one, and it is antisymmetric in  $\theta$ . Thus no net contribution to  $K_1$  will be made by a symmetrical distribution of Mode-II dislocations.

Figure (51b) shows the shielding of a dislocation in a pure Mode-II configuration as a function of angle  $\theta$ .

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When a Mode-II crack interacts with a symmetric pair of dislocations in a Mode-I configuration (Fig. 50a), all three terms contribute in Eq. (38.1), because the Burgers vector has both  $x_1$  and  $x_2$  components. However, the firstterm contribution is zero because  $(b_1)_{x_1} = -(b_2)_{x_1}$ . The second term is an odd function of  $\theta$ , and hence one dislocation again cancels the other. The third term also contributes zero because  $(b_1)_{x_1} = -(b_2)_{x_1}$  and the angular function is an even function of  $\theta$ . Mode III is essentially "orthogonal" to the other two modes, and no crossover terms occur.

The overall result is thus that, so far as shielding is concerned, there are no significant cross terms in the shielding contributions, and the modes can be considered individually. This result, of course, depends on the assumption of symmetry. When a single dislocation is being emitted from a Mode-I crack, then there is a contribution to  $K_{II}$ , and a reaction in Mode II. This point is further discussed in Part VII,39.

The most interesting mixed-mode crack is one where sufficient Mode 1 exists to ensure that the crack develops an open surface on the crack plane, but where the primary loading is Mode III (the "Ohr" configuration of Fig. 13) or Mode II. In pure Mode II or III, of course, the bonds are not separated across the crack plane, and no physical crack exists, as discussed in Part VI,28. Suppose initially, then, that a sharp stable Mode-I crack exists so that the Griffith relation is satisfied at the crack tip,

$$k_{\rm I}^2 = 4\gamma(1-\nu)/\mu. \tag{38.2}$$

No dislocations are presumed present initially. As Mode-II loading is applied, the local  $k_{\mu}$  starts from zero and increases. Because of the elastic linearity of the Mode-I and -II stress states, the Mode-I stress is not changed by the Mode-II loading. As noted in Part VI,28, the fracture criterion at the tip is slightly modified, because the bonds at the tip will be sheared, and in general, less  $k_i$  will be required to hold the atoms open there. However, we expect this effect to be small, as proposed in Part VI.28. Thus, as k<sub>n</sub> is increased, no additional cleavage occurs, but Mode-II loading can induce dislocation emission, and the standard dislocation emission conditions of Part VI on the crack plane will be valid. We now presume that the crack plane is a slip plane. and the standard one-dimensional dislocation distribution of edge dislocations will be generated, controlled by the local emission criterion in Mode II and the total externally applied  $K_{\rm H}$ . In this mixed-mode case, the Mode-II dislocations exert little shielding on  $K_1$  of the crack, as explained earlier in this section. So long as the Mode-I-type dislocations are not produced by either emission or external source activiation, the crack can cleave at very low  $k_1$ values, yet generate an indefinite number of Mode-II dislocations with large amounts of plasticity. Thus in this mixed-mode case, high ductility and cleavage comfortably coexist.

Lynch<sup>132</sup> has in fact observed phenomena very similar to that described above in chemically embrittled metals. In his experiments, the external chemical environment presumably modifies the Griffith criterion through its effect on y so that a cleavage crack is stable. Large amounts of deformation are then observed close to the cleavage plane, as described above for emission in Modes 11 and 111. These ideas suggest in practice cleavage fracture should commonly exhibit this type of shear-mode emission because of the difficulty of ensuring pure Mode-1 loading.

An important proposal has been made by Sinclair and Finnis<sup>89</sup> that the cleavage/emission balance can be altered after emission of a group of dislocations has occurred. Their proposal is built on a cleavage criterion like Eq. (28.8) and an assumption that emission occurs in Mode I in an asymmetric manner so that mixed loading at the tip occurs. We have argued that Eq. (28.8) is not the correct cleavage criterion, but there remains the issue mentioned in Part VI,28, where cleavage and emission are finely balanced against one another, that mixed-mode loading might still alter this balance. Indeed, in the "Ohr" configuration of Fig. 13, a small and presumably stable Mode-I crack is observed as schematically shown in Fig. 47. This crack does not emit in the Mode-I configuration of Fig. 50a, as demonstrated in the electron micrograph of Fig. 13, even though the material is the supposedly intrinsically ductile metal, copper, where stable Mode-I cracks are not supposed to exist in pure Mode I. This result has not been analyzed yet in terms of the available slip system geometry and stress state in the films. Two possibilities exist. The first is that some Mode-II loading exists of sign and magnitude sufficient to raise the emission criterion from Eq. (28.2) relative to the cleavage criterion, and the second is that the Mode-III loading changes the cleavage/emission balance at the crack tip. This is an important issue, and requires further study.

Having explored shielding effects on the crack, we turn now to some theorems regarding the forces experienced by the dislocations. The first theorem which can be proved is that in Mode I, for two symmetrically placed dislocations with the configuration of Fig. (50a),

$$(f_{dd'})_{\text{hip plane}} = 0. \tag{38.3}$$

The second theorem of interest relates to the relation (15.10). In the deformation theory of cracks using the *J* integral, it is shown that in the limit of small-scale yielding where the region of deformation is small compared with the crack size and the specimen size, the force on the total configuration is given by the generalization of Eq. (15.10); that is,

$$\operatorname{Re}(\bar{f}_{\operatorname{ten}}) = \frac{(K_1^2 + K_{11}^2)}{2\mu}(1 - \nu) + \frac{K_{111}^2}{2\mu}.$$
 (38.4)

This theorem is also valid when the deformation field is composed of singular dislocations. The reason is that the far-field asymptotic form of the stress in Mode III and the potential functions in plane strain are all dominated by the  $1/\sqrt{z}$  term given by the far-field K field in each case. (See Eqs. (10.3), (10.11), and (10.12).) The next term in the expansion at infinity is not the simple

<sup>&</sup>lt;sup>132</sup> S. P. Lynch, AIME Symp. Liquid Metal Embrittlement (1983).

dislocation term in  $1/\sqrt{z}$ , but a higher-order term in  $1/\sqrt{z^3}$ . In the limit of large |z|, the integration of these  $z^{-3/2}$  stresses around a contour where  $|z| \gg |\zeta_j|$  on the contour  $(\zeta_j$  is the position of any shielding dislocation) in either the J-integral expression, or the Eshelby theorem [Eq. (14.8)], contributes a zero contribution to f. The reason, of course, is the image that the dislocation develops in the open crack which cuts off its long-range 1/z field.

Using, Eq. (38.3) and the shielding results of Eqs. (15.6) and (16.7), some simplification in the force equations is possible. Writing

$$K = k + K_{\rm D}, \tag{38.5}$$

which will be valid for each mode, then for each mode.

$$\operatorname{Re}(\bar{f}_{iot}) = \operatorname{Re} f_{e} + \operatorname{Re} \sum_{j} (f_{d})_{j} = \frac{K^{2}}{2\chi},$$

$$\chi = \begin{cases} \mu & \text{Mode III} \\ \mu/(1-\nu) & \text{Mode I, II.} \end{cases}$$
(38.6)

Using Eq. (38.5), Eq. (38.6) becomes

$$\operatorname{Re}\sum_{j}(f_{d})_{j} = \frac{KK_{D}}{\chi} - \frac{K_{D}^{2}}{2\chi}.$$
(38.7)

Since the first term is linear in K, it represents the direct force term on the dislocations, while the second term is the combination of image and dislocation-dislocation interactions. Using the shielding relations, Eqs. (15.6) and (16.7), these become in turn for each dislocation

$$\operatorname{Re}(f_{cd})_{tot} = K_{tt}b_{3}\operatorname{Re}(1/\sqrt{2\pi\zeta_{j}}), \quad \text{Mode III}$$

$$\operatorname{Re}(f_{cd})_{tot} = \frac{+K_{1}}{\sqrt{2\pi r_{j}}} \left[ b_{2j}\cos\frac{\theta_{j}}{2} + \frac{\sin\theta_{j}}{2} \left( b_{1j}\cos\frac{3\theta_{j}}{2} + b_{2j}\sin\frac{3\theta_{j}}{2} \right) \right], \quad \text{Mode I}$$

$$\operatorname{Re}(f_{cd})_{tot} = \frac{K_{1}}{\sqrt{2\pi r_{j}}} \left[ b_{1j}\cos\frac{\theta_{j}}{2} - \frac{\sin\theta_{j}}{2} \left( b_{1j}\sin\frac{3\theta_{j}}{2} - b_{2j}\cos\frac{3\theta_{j}}{2} \right) \right], \quad \text{Mode II}$$

$$(38.8)$$

The term in  $K_D^2$  is a double sum over the dislocation distribution. The terms in  $b_j b_i$  represent dislocation-dislocation interactions. The  $b_j^2$  term represents the self-image term. These expressions are not written here, but are explicit manifestations of the more general expressions in Eqs. (16.13) and (16.16), which can be useful.

In the only serious attempt at Mode-1 shielding calculations to date, the BCS model has been extended by Riedel<sup>133</sup> and Vitek<sup>134</sup> to the Mode-I crack with a pair of slip planes intersecting the crack tip at an angle of  $\pm \theta$ . The resulting singular integral can be converted to one of Fredholm type which can be numerically integrated. The numerical results compare in all major aspects to the full two-dimensional continuum plastic-deformation theory results; so the approximation that slip only occurs on two symmetrically oriented slip planes is apparently a good one. This work, however, did not include considerations of the local k and local crack equilibrium. The results suggest that including such a dislocation-free zone in these calculations would lead to a quite satisfactory description of shielding in Mode I, and hence to a realistic toughness relation. Sinclair<sup>135</sup> has carried the problem one step further, and made a numerical calculation for a wedge crack created by emission of a symmetrical distribution of dislocations on symmetrical slip planes making angles of  $\pm \theta$  to the symmetry plane of the wedge. In all these cases, one of the important results is the generation of a maximum dilatation at some distance ahead of the crack tip, which is thought to be correlated with the generation of new cracks in the hole-growth model.

## **39. GROWING CRACKS**

A growing crack differs from a static one in two important respects. A growing crack has a past history in the sense that its deformation zone has passed through the specimen and left behind a wake of work-hardened material extending some distance on either side of the open flanks of the crack. Secondly, a growing crack is also a time-dependent phenomenon, and will involve rate-dependent dissipation processes in any plastic response of the material, and may also involve dynamic or inertial effects as well. Both of these aspects of moving cracks lead to important physical effects different from static cracks.

#### a. Quasistatic Cracks

In the quasistatic case, inertial effects are neglected. Hart <sup>103</sup> has treated this problem in an elegant approach using a continuum (but two-dimensional) form of the shielding theory in Mode III. In his work, the crack is assumed to move with constant velocity, and the dislocation density is generated by a

<sup>133</sup> H. Riedel, J. Mech. Phys. Solids 24, 277 (1976).

<sup>134</sup> V. Vitek, J. Mech. Phys. Solids 24, 67, 273 (1976).

<sup>135</sup> J. Sinclair, Nucl. Metall. 20, 388 (1976).

deformation-rate constitutive law which is consistent with laws describing creeping materials, but is not a strain-hardening law. In his earlier work, the deformation zone is also assumed to move with the crack, and the problem of the wake is not addressed. In later work, yet to be published, however, the wake is included, so that a true dissipation takes place. The feature of Hart's work which will be familiar to the reader of this article is that a local k is derived. For a moving crack, even in a continuum theory, this is possible so long as the creep deformation near the crack tip is sufficiently slow so that the crack tip is not completely shielded. This requirement becomes an assumption for Hart's treatment, and it turns out to be attainable provided the creep law,

$$\dot{\epsilon} = A\sigma^* + \dot{\sigma}/\mu, \qquad (39.1)$$

in the vicinity of the tip has an exponent, n < 3 and far from the crack tip, n > 3. Hui and Riedel<sup>136</sup> have published a general analysis of the asymptotic forms of the stress fields at the crack tip and at large distances with creep laws of the form of Eq. (39.1). When n > 3 near the crack tip, no k field is possible, and the field is dominated by the plasticity. That is, the crack tip is essentially fully shielded, even though it has a stress singularity.

The interesting predictions of Hart's analysis are that (1) the crack must have a finite velocity, or the creeping material at the crack tip will completely shield the tip and destroy the crack k field, and (2) that for high velocities a breakaway phenomenon occurs corresponding to the crack outrunning the ability of the material to form a significant shielding charge of B argers vector. In the analysis, this breakaway actually corresponds to an analytically doublevalued solution (Fig. 52).

The work of Hart and of Hui and Riedel is of considerable interest, because it shows that, when the crack is moving, rate-dependent continuum solutions can be constructed which are not limited by the Rice theorem  $^{32,46}$  discussed in the introduction, Part VII,32. When  $v \rightarrow 0$ , as Hart shows, the creeping material at the crack tip will eventually damp out any static stress concentration, and the k field will be destroyed. Then no atomic-bond-breaking process at the tip can be invoked, because at best the stress field is restricted to the much lower stresses allowed by deformation processes, and Rice's theorem applies. When v is greater than some critical value, and when n < 3, then the plastic creep does not have time to fully shield an atomically sharp crack when it moves into a new region of the material. Then a local k can be sustained, and the bond-breaking stresses at the tip can be achieved. But if n > 3, then these results are no longer possible, and the atomic crack breaks down. One might say the physical reason for this breakdown is that the condition described in Part VII,33 leading to Fig. 44 obtain, and Rice's theorem takes over.



FIG. 52. Predicted form of K(v) for a creeping crack after Hart.<sup>103</sup> The curve stops at the lower limit for v and has a branch with negative slope corresponding to dynamically unstable states.

These rate-dependent results for moving cracks are closely related to the general point of view of this article, that conditions in the near tip region of a crack involving the distribution of dislocation sources and their ease of operation determine whether the sharp crack can be sustained. The condition n < 3, physically, is another statement of the same general type. Indeed, as we will show below, one can derive some analogous moving-crack behavior on the basis of the shielding ideas developed here in Part VII,34.

Imagine that a brittle crack is moving at velocity v, and that a dislocation cloud has been attached to the crack by some prior event which will not enter further into the analysis. Suppose the slip plane for the dislocation is parallel to the crack plane, that the Mode-III analysis applies, and that the entire configuration is in steady-state motion with velocity v. With the use of Eqs. (34.8)-(34.10), the configuration is consistent with a steady-state velocity if the friction stress is determined by the stress-velocity law for the dislocations,  $\sigma_i(v)$ . For a given B, and K, the size of the pileup, d, is determined by Eq. (34.10). The velocity is then determined by Eq. (34.9). Equation (34.8) is a relation between k and c, because all the other parameters in Eq. (34.8) have been determined by the external conditions or by Eqs. (34.9) and (34.10). Thus if the crack local k is a function of v, or in a quasistatic limit simply given by the Griflith relation,  $k^2 = 4\mu y$ , Eq. (34.8) sets c so this local k can be maintained. Hence a K(v) law is generated consistent with the dislocation  $\sigma_i(v)$  law and the

<sup>&</sup>lt;sup>134</sup> C. Y. Hui and H. Riedel, Int. J. Fract. 17, 409 (1981).

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shielding relations for all velocities v. However, unless the dislocation slip planes are exactly coincident with the crack plane, there is a lower limit to c, and a maximum limit to K or v. This configuration is shown in Fig. 53, and is due to the fact that when the closest dislocation is on a slip plane a distance  $c^*$ above or below the crack plane, the lower limit of c in Eq. (34.8) is  $c^*$ . For kvalues above this initial point, the shielding of the crack tip "runs out of steam," and the crack breaks away from its dislocation shield.

An actual physical situation approximating the above description is that found in LiF in early experiments on dislocations interacting with cracks by Burns and Webb.<sup>137</sup> In their case the slip planes of the dislocations were inclined to the plane of the crack (in the  $x_3$  direction), so that the dislocations wrapped around the crack to form a hairpin shape. The limiting value of c in this case would correspond to the distance between neighboring dislocations in the  $x_3$  direction, and  $\sigma_t$  would be the sum of the actual  $\sigma_t$  for the part of the dislocations looping around the crack and the line tension of the straight segment forming the wake. The interpretation and analysis originally given by Burns and Webb is not inconsistent with this picture, and their experimental results showed the kind of breakaway proposed above.

If, on the other hand, the crack generates new dislocations from sources in the medium as it moves along, a shielding charge is built up and then left behind as a wake as the crack moves on. Speaking physically, the shielding charge generated would again lead to relations between the external K,  $\sigma_r$  (or yield stress), and the size of the deformed region satisfying Eqs. (34.9) and (34.10) provided the system is steady state. Again, the conditions on the local k would involve the distance to the first shielding dislocation. This distance will always be greater than zero, because sources of dislocations are always distributed in the bulk matrix on a very heterogeneous scale. Since k is determined by this close-in dislocation distribution for steady-state shielding, there will again be a limiting lower bound for c associated with the dislocation

<sup>137</sup> S. J. Burns and W. W. Webb, J. Appl. Phys. 41, 2078, 2086 (1970).

source distribution. Since B is a decreasing function of V because of the rate dependence of dislocation generation, there will always be a limiting velocity where the required shielding at the crack tip cannot be achieved, and the crack will break away from its shielding charge.

Thus the shielding relations of Part VII,34 lead to the same breakaway physics as Hart's continuum analysis. However, the shielding relations show that the breakaway is intimately connected with the dislocation structure close to the crack tip, whereas the physical basis for breakaway is less clear in Hart's analysis.

The prediction by Hart that the crack will be completely shielded in the creep regime at very low velocities so that stationary cracks are impossible is a statement which should be taken seriously for some cases. It suggests that a material can behave in a brittle way for sufficiently high strain rates, but blunt out any brittle crack at low strain rates by deformation in the bulk. Materials which are brittle at room temperature (even though some deformation may be present), but ductile at very high temperatures for ordinary testing machine strain rates, suggest this behavior. On the other hand, of course, there are many cases where a static description of a shielded stationary crack is a valid picture.

The discussion of this subsection raises an important property of moving cracks, namely that when shielding dislocations are present, and the crack moves, then a wake is left behind as the crack moves. For purposes of modeling the toughness of the material, the existence of the wake is a crucial factor, because it represents a part of the dissipation, and it contributes to the overall stress. Hart has dealt with this term in an analytic way in work yet unpublished for the Mode-III continuum solution, but Hirth *et al.*, <sup>138</sup> and Thomson and Sinclair <sup>33</sup> also discuss the problem from the standpoint of the forces on the total configuration. This problem has also been extensively investigated in the continuum plasticity approximation.<sup>139</sup>

#### b. Inertial Effects

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The mathematics of time-dependent crack motion is subtle and fascinating. This result will not be surprising to those familiar with the analysis for dynamic dislocations.<sup>20</sup> For a recent review of the elastic problem, the reader is referred to an excellent paper by Freund.<sup>140</sup>

The steady-state stress problem is relatively easy to solve, and complex function methods quite similar to those of Part III lead to the result that the

134 J. P. Hirth, R. G. Hoagland, and C. H. Popelar, Acta Metall. 32, 371 (1984).

139 J. Rice, in "Mechanics of Solids" (H. Hopkins and M. Sewell, eds.), p. 539. Pergamon, Oxford, 1982.

149 L. B. Freund, Mech. Today 3, 55 (1976).

moving crack is again characterized by a K field, but that the value is decreased by comparison to the static value. Thus

$$K(v) = \sqrt{\frac{2}{\pi}} h(v) \int_{0}^{vt} (vt - x)^{-1/2} \sigma(x) dx, \qquad (39.2)$$

in complete analogy to the static semi-infinite crack, but where h is a nearly linear function of v given in Fig. 54 for Mode I. In Mode III, the Lopentz contraction comes into play on the displacement and stress functions in the expected way on the x axis. Thus, the complex function,  $\eta(z)$ , of Eq. (8.2) becomes

$$\eta(x - vt) = \left(\frac{1 - v/c}{1 + v/c}\right)^{1/4} \eta_0 \left(\frac{x - vt}{\sqrt{1 - v^2/c^2}}, y\right), \quad (39.3)$$

where  $\eta_0$  is the static crack function and c is the shear sound speed. In this case, the function h(v) becomes simply

$$h(v) = \left(\frac{1 - v/c}{1 + v/c}\right)^{1/4} \left(1 - \frac{v^2}{c^2}\right)^{1/4}.$$
 (39.4)

Further, the instantaneous force on the crack tip can be found (140) and is given in Mode I by the result

$$f = (K_0^2/E)(1 - v^2)g(v), \qquad (39.5)$$

where  $K_0$  is the static value of  $K_1$  and g(v) is again shown in Fig. 54. This result states that, when a fracture criterion such as f = 2y is given and y is a constant, then the external load as specified by  $K_0$  must be increased to supply the energy to open the crack surface. The extra energy input is, of course, put into the radiation field of the crack.



FKi. 54. Functions g(v) and h(v) for Eqs. (39.5) and (39.2).

The startling result for non-steady-state motion is that an elastic crack has no inertia. As a source of stress in a medium governed by a wave equation, one would expect a radiation resistance inertia for the crack such as exists for the classical electron and for the dislocation.<sup>20</sup> In Mode III, the solution has been discussed by Eshelby, and in an elegent paper,<sup>141</sup> he shows that the lack of inertia follows from the fact that the Mode-III crack solution is a "distortionless" solution of the wave equation. That is, a general solution of the wave equation in two dimensions exists of the form

$$\sigma = \frac{1}{z^{1/2}} f(r \pm ct), \qquad (39.6)$$
$$z = re^{i\theta},$$

from which a crack solution can be constructed for arbitrary motion. The characteristic crack  $1/z^{1/2}$  function is thus a fundamental form for the twodimensional wave equation. The result which can be constructed easily from Eq. (39.6)—and the argument is almost transparent from Eq. (39.6)—is that a crack can be stopped suddenly from a state of uniform motion, and the precise steady-state stress distribution is radiated out from the center with velocity c. Since the radiated solution is precisely the static solution, no radiation resistance is exerted on the crack. This surprising result is true even though the crack is equivalent to a virtual dislocation distribution over the cleavage surface, and these dislocations, singly, do possess an inertia. The point is that the coherent interaction between the crack dislocations cancels the inertia of the collective motion when they move as a crack.

Freund has shown<sup>140</sup> that the full static solution is not radiated when a crack is stopped similarly in plane strain (Mode I or II) for all angles. However, the static solution is generated along the crack line in front of the crack, and this is sufficient for the Mode-I and Mode-II cracks to possess zero inertia also.

The foregoing results are valid only for semi-infinite cracks. Freund shows that for finite cracks interactions between the crack tips modify the non-steady-state character of crack motion in an essential way.<sup>140</sup>

## 40. TIME-DEPENDENT CLEAVAGE/EMISSION CONSIDERATIONS

There has already been occasion to note that several cases exist where brittle cleavage cracks appear to be observed running at high speed in materials which are demonstrably ductile in the sense of the criterion, Eq. (28.5).

<sup>&</sup>lt;sup>141</sup> J. D. Eshelby, in "Physics of Strength and Plasticity" (The Orowan 65th Anniversary Volume, A. Argon, ed.), p. 263. MIT Press, Cambridge, Mass., 1969.

Pugh<sup>142</sup> has shown that a crack in brass started at an embrittled site is able to propagate for a distance of the order of tens of micrometers in fast cleavage before coming to rest. There are similar findings in pure copper under corrosion conditions.<sup>143</sup> After nucleation at sites in dislocation cell boundaries, Wilsdorf finds that fast cleavage occurs in foils of copper and gold under stress for distances of the order of a few to 10 micrometers.<sup>6</sup> Ohr *et al.*<sup>10</sup> report that cleavage is initiated in Al in the configuration of Fig. 13 and again runs as a fast cleavage crack through the foil for a distance of micrometers before arrest. Gerberich<sup>144</sup> has shown that cracks in Fe/Si single crystals can be made to propagate as cleavage cracks at high velocities with some, but small dislocation activity, whereas stationary cracks in this material take the wedge shape, according to Vehoff and Rothe.<sup>99</sup> The observations in thin films may be affected by the thin-film geometry, e.g., by rapid slideoff, but the results in thicker specimens are not subject to this objection.

These results suggest that the competition between cleavage and emission is velocity dependent, and proposals along this line have been made by various authors. Jokl et al.<sup>145</sup> proposed a model of combined emission and cleavage, where shielding of the crack plays a part in the emission criterion. Rather crude assumptions are made, however, about the basic mechanisms competing at the crack tip. Knott<sup>146</sup> has proposed a very interesting model for virtual dislocation emission, in which an emitted dislocation falls back into the cleavage surface after the crack moves on. Such a mechanism would lead to an enhanced effective y for a fast-moving crack, because of the energy dissipation of dislocations popping in and out of the crack, but would yield a clean cleavage crack as a result. Paskin et al.63 have simulated fast moving cracks in materials which are ductile for static cracks, and the cleavage is clean. On the other hand, a paradox exists, because if a crack has zero inertia, an emitted dislocation will stop the crack. Once stopped, of course, by postulate, the crack will simply emit dislocations as the stress builds up. Thus, an adequate understanding of the dynamic crack-dislocation interaction does not yet exist.

#### Appendix

In this appendix, some essential basic mathematics of elasticity is collected. The Appendix is in three parts. In the first, the governing equations for plane

- <sup>142</sup> E. N. Pugh, in "Atomistics of Fracture" (R. Latanision and J. Pickens, eds.), p. 997. Plenum, New York, 1983.
- 143 K. Sieradsky, R. Sabatini, and R. Newman, Met. Trans. A 15, 1941 (1984).
- 144 W. Gerberich, unpublished results.

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145 M. Jokl. V. Vitek, and C. J. McMahon, Acta Metall. 28, 1479 (1980).

<sup>146</sup> J. Knott, in "Atomistics of Fracture" (R. Latanision and J. R. Pickens, eds.), p. 209. Plenum, New York, 1983. (A.1)

strain are developed in terms of the Goursat potential functions. In the second, a generalized conformal-mapping analysis for these functions is developed. In the third part, the mathematics relevant to the use of Muskhelishvili's singular integrals is presented.

## I. PLANE-STRAIN FIELD EQUATIONS

The mathematical development of this and the following section is based on papers by Stevenson,<sup>147</sup> and Tiffin,<sup>148</sup> but some of the same results will be found in the Muskhelishvili treatise.<sup>13</sup> In plane strain, the displacement  $u_i$  satisfies and  $u_3 = 0$ . u will be taken to be a complex vector

and

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$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial z} + \frac{\partial}{\partial \overline{z}}; \qquad \frac{\partial}{\partial x_2} = i \left( \frac{\partial}{\partial z} - \frac{\partial}{\partial \overline{z}} \right)$$

 $u = u_1 + iu_2$ 

Derivatives of u (which is not yet assumed to be analytic) are given by

$$2\frac{\partial u}{\partial z} = \theta + 2i\mathscr{W}, \quad \theta = u_{i,i}; \quad \mathscr{W} = \frac{1}{2}(u_{i,j} - u_{j,i}). \quad (A.2)$$

 $\theta$  is the dilatation, and # the rotation. The equilibrium equations (7.1) become

$$\sigma_{11,1} + \sigma_{12,2} = 0,$$
  

$$\sigma_{22,2} + \sigma_{12,1} = 0.$$
(A.3)

Multiplying the second equation by i and adding yields

$$\frac{\partial}{\partial z}(\sigma_{11}-\sigma_{22}+2i\sigma_{12})+\frac{\partial}{\partial \bar{z}}(\sigma_{11}+\sigma_{22})=0 \tag{A.4}$$

This equation states the condition for the existence of a potential function F, such that with Eqs. (A.1) and (7.2),

$$\frac{\partial F}{\partial \bar{z}} = \sigma_{11} - \sigma_{22} + 2i\sigma_{12} = 4\mu \frac{\partial u}{\partial \bar{z}}, \qquad (A.5)$$

$$\frac{\partial F}{\partial z} = \sigma_{11} + \sigma_{22} = 2(\lambda + \mu)\theta. \tag{A.6}$$

A. C. Stevenson, Proc. R. Suc. London Ser. A 184, p129, p218 (1945).
 R. Tiffen, Q. J. Mech. Appl. Math. V, 352 (1952).

Equation (A.5) is immediately integrable to give .

$$4\mu u = f(z) - F(z, \bar{z})$$
 (A.7)

Substituting Eq. (A.2) into (A.6) gives

$$\frac{1}{2(\lambda + \mu)}\frac{\partial F}{\partial z} = 2\frac{\partial u}{\partial z} - 2i\mathcal{W}$$
 (A.8)

From Eq. (A.6), because  $\theta$  is real,  $\partial F/\partial z$  is real, and Eq. (A.8) is also real. Hence, substitution of Eq. (A.7) into (A.8) leads to

$$\frac{\partial F}{\partial z} = \frac{\lambda + \mu}{2(\lambda + 2\mu)} \left[ \frac{\partial f}{\partial z} + \left( \frac{\overline{\partial f}}{\partial z} \right) \right] = 2\varphi'(z) + \overline{\varphi'(z)}. \tag{A.9}$$

The function  $\varphi'$  is defined by Eq. (A.9). This equation is now integrable, giving

$$f'(z, \bar{z}) = 2[\varphi(z) + z\varphi^{*'}(\bar{z})] + 2\psi^{*}(\bar{z}).$$
 (A.10)

The star operator is defined by

$$\varphi^*(z) = \overline{\varphi(\overline{z})}, \quad \text{etc.} \quad (A, [1])$$

and is a convenient way to show explicitly that  $\overline{\varphi}$  and  $\overline{\psi}$  are functions of  $\overline{z}$ , not z.

Now Eqs. (A.5), (A.6), and (A.7) take the form

$$\sigma_{11} + \sigma_{22} = 2[\varphi'(z) + \overline{\varphi'(z)}], \qquad (A.12)$$

$$\sigma_{22} - \sigma_{11} + 2i\sigma_{12} = 2[\bar{z}\varphi''(z) + \psi'(z)], \qquad (A.13)$$

$$2\mu u = \kappa \varphi(z) - z \overline{\varphi'(z)} - \overline{\psi(z)},$$
 (A.14)

 $\kappa = 3 - 4\nu$  (plane strain). (A.15)

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Equations (A.12)-(A.15) are the new field equations of plane-strain elasticity. They are expressed in terms of the two independent complex functions,  $\varphi(z)$ and  $\psi(z)$ , even though the stresses and the displacement functions are not necessarily complex functions of z. If the displacement is a single-valued function of z (and perhaps  $\overline{z}$ ), then the elastic problem automatically satisfies the incompatibility equations discussed in all elasticity books. In the form of the theory used here, however, they need not be addressed explicitly. For example, if dislocations are present as singularities, then  $\varphi'$  and  $\psi'$  have poles at the position of the dislocation, and the u function is multivalued there, with

$$\Delta u \Big|_{x \neq \zeta} = b = b_1 + ib_2. \tag{A.16}$$

We will not consider continuous distributions of dislocations, but in that case,

the appropriate Burgers-vector density function can be defined. The functions  $\varphi$  and  $\psi$  are the standard potential functions of Goursat,<sup>149</sup> e.g., as used in Muskhelishvili.<sup>15</sup> In plane strain, the Burgers vector defined by Eq. (A.3) corresponds to an edge dislocation with components  $b_1$  and  $b_2$ , and to a crack in either Mode 1 or Mode 11.

The general elastic solution, combining antiplane strain with plane strain, with a screw component of a Burgers vector as well as edge components, and including mixtures of Modes I, II, and III, is a simple linear combination of stresses and displacements calculated from the three independent potential functions,  $\eta(z)$ ,  $\varphi(z)$ , and  $\psi(z)$  with stresses and displacements given by Eqs. (8.1) and (8.2) and (A.12)-(A.15).

Generally speaking, since  $\varphi$ ,  $\psi$ , (and  $\eta$ ) are complex functions, solutions are obtained for an elastic problem by applying considerations of analyticity and function theory to the potential functions in the light of the boundary conditions set on the problem by the existence of free surfaces, behavior of stress at  $\infty$ , multivaluedness of u, etc.

## 2. CONFORMAL MAPPING

One of the important ways to solve two-dimensional boundary value problems is by means of conformal mapping, in which complicated problems are transformed into simpler soluble ones. The same is true of elastic problems, except that in this case, since tensors are involved, the analysis must be generalized beyond that familiar in electrostatics or hydrodynamics.

Consider a coordinate transformation which maps the z plane (the initial problem) into the  $\xi$  plane (the simpler problem) and the real coordinates,  $x_1$ ,  $x_2$ , into the new coordinates,  $y_1, y_2$ . In real coordinates the transformation law from the tensor  $A_{ij}(x_1, x_2)$  into the new tensor  $A_{ij}(y_1, y_2)$  is given in standard notation

$$A'_{pq\cdots}(y_1, y_2) = \beta_{pi}\beta_{qj}\cdots A_{ij\cdots}(x_1, x_2),$$
  

$$\beta_{pi}\beta_{pj} = \delta_{ij},$$
  

$$dx_i = \sum_j \frac{\partial x_i}{\partial y_j} dy_j = \sum_j h_{(i)}\beta_{ij} dy_j.$$
  
(A.17)

Here the  $\beta$  are the rotation matrices, and the tensors are not separated into their contra- and convariant parts. The advantages of this form of the transformation law is that stress tensors do not change their dimensional

149 E. Goursat, Bull. Soc. Math France 26, 236 (1898).

units when transformed into a new coordinate system. (See Morse and Feshbach<sup>150</sup>.) The  $\beta$  are functions of position in general.

A rotation suitable for transforming vectors and tensors which are complex functions is now required. If the mapping of z into  $\xi$  is given by the functional relationship

$$z = z(\xi), \qquad (A_1 t_R)$$

then the rotation angle  $\alpha$  of the  $x_1$  coordinate into the  $y_1$  coordinate at the position z is given by

$$z = \left| \frac{dz}{d\xi} \right| e^{i\epsilon} d\xi, \qquad (A.19)$$

and the transformation law Eq. (A.17) for a complex vector A(z) into the new vector  $A_T(\xi)$  is given by

$$A_{\rm T}(\xi) = e^{-i\alpha} A(z).$$
 (A.20)

A problem in notation arises here, because the standard notation for a transformed quantity is the prime as used in Eq. (A.17). In the complex plane, however, the prime will be reserved for differentiation with respect to a complex variable. Hence the subscript T will be used to denote a transformed quantity. Since z' in general is a function of position, the rotation angle varies also with position z. The reader is also reminded that the functional form of  $A_T(\xi)$  is recovered from the substitution

$$A_{\rm T}(\xi) = A_{\rm T}(\xi(z)) = A(\xi(z))e^{-i\alpha} = A(z)e^{-i\alpha}.$$
 (A.21)

In this article, it will be implied that when the new coordinate  $\xi$  is used as an independent variable in a function f, the functional form is defined by  $f(\xi) \equiv f(z(\xi))$ .

Transformation laws can now be written for the relevant elastic quantities. In antiplane strain, relative to rotation in the  $x_1$ ,  $x_2$  plane,  $u_3$  is a scalar quantity. Also  $\sigma_{3j}$  relative to the same rotation transforms as a vector. However, since the complex "vector" defined in Eq. (8.2) is related to the complex conjugate of the "true" vector  $\sigma_{3j}$ , the function transforms as follows.

a. Antiplane Strain

$$u_{\rm T}(\xi) = u(z(\xi)) = u(z),$$
 (A.27)

$$\sigma_{\rm T}(\xi) = e^{i\alpha}\sigma(\xi(z)) = e^{i\alpha}\sigma(z). \tag{A 23}$$

In plane strain the following relations hold.

<sup>130</sup> P. Morse and H. Feshbach, "Methods of Theoretical Physics," Vol. I, p. 21. McGraw-Hill, New York, 1953. b. Plane Strain

$$(\sigma_{11} + \sigma_{22})_{T} = \sigma_{11} + \sigma_{22}, \qquad (A.24)$$

$$(\sigma_{22} - \sigma_{11} + 2i\sigma_{12})_{T} = e^{2i\alpha}(\sigma_{22} - \sigma_{11} + 2i\sigma_{12})$$

$$= \frac{z'(\xi)}{\overline{z'(\xi)}}(\sigma_{22} - \sigma_{11} + 2i\sigma_{12}), \qquad (A.25)$$

 $u_{\mathrm{T}} = e^{-u}u. \tag{A.26}$ 

The first of these equations follows because the contracted stress tensor is a scalar, the second is from direct substitution in the tensor transformation laws, and the third because  $u = u_1 + iu_2$  is a true complex vector.

With these transformation laws, the transformed elastic field equations become of the form following.

c. Antiplane Strain

$$T_{T}(\xi) = \frac{2}{\mu} \operatorname{Im}[\eta(z)] = \frac{2}{\mu} \operatorname{Im}[\eta(z(\xi))],$$
 (A.27)

$$\sigma_{\rm T} = e^{i\alpha}\sigma(z) = 2e^{i\alpha}\frac{d\eta}{dz} = 2e^{i\alpha}\frac{d\xi}{dz}\frac{d\eta(z(\xi))}{d\xi} \tag{A.28}$$

d. Plane Strain

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$$(\sigma_{11} + \sigma_{22})_{\mathrm{T}} = 2[\varphi'(z) - \overline{\varphi'(z)}] = 2[\Phi(\xi) + \overline{\Phi(\xi)}], \qquad (A.29)$$

$$(\sigma_{22} - \sigma_{11} + 2i\sigma_{12})_{T} = 2e^{2i\alpha} \left( \frac{z(\xi)}{z'(\xi)} \Phi'(\xi) + \Psi(\xi) \right)$$
$$= 2 \left( \frac{\overline{z(\xi)}}{z'(\xi)} \Phi'(\xi) + \frac{z'(\xi)}{z'(\xi)} \Psi(\xi) \right),$$
(A.30)

$$2\mu u_{\rm T} = e^{-ie} [\kappa \varphi(z(\xi)) - z(\xi) \Phi(\xi) - \overline{\Psi(z(\xi))}]$$
(A.31)

$$\mathsf{P}(\xi) = \frac{d\varphi(z(\xi))}{d\xi}; \qquad \varphi(z) = \varphi(z(\xi)) = \int z'(\xi) \Phi(\xi) d\xi, \quad (A.32)$$

etc. In these equations, the derivatives of the potentials in the  $\xi$  plane are awkward to handle, so for both  $\varphi$  and  $\psi$ , the capital functions  $\Phi$  and  $\Psi$  are defined in Eq. (A.32).

The strategy in the use of the conformal-mapping procedure for Eqs. (A.27)-(A.32) is to map the original complicated boundary into a simpler geometry, e.g., a wedge into a half-plane, etc., and solve the new transformed boundary problem in the simpler geometry. There is a "trap" in this strategy, however, when a mapping function is used where the scale factor h is not unity,

then the two coordinate systems are not physically equivalent, since the scale of length is different in the two. Hence, a comparison of two *a priori* solutions in two such coordinate systems without considering the scale factor for length measurements between the two systems will lead to error. For this reason, the strategy here will always be to express the physical problem in the "natural" coordinate system, and use the  $\xi$  system only as a mathematical convenience in handling the geometry of the boundary conditions. Note also that in this spirit the potential functions corresponding to the z system are used, exclusively, without ever writing down the transformed potentials. The relations between  $\varphi, \psi$ , etc., and the transformed displacements and stresses are, of course, given by Eq. (A.27)-(A.32). When these potentials are written in terms of the new coordinates  $\xi$ , however, it does not mean the new functions are then the new transformed potentials, which would relate to the new stresses by relations such as Eqs. (A.12)-(A.15), etc.

In order for this strategy to work conveniently, it must be true that the boundary conditions are "covariant." That is, if on the initial boundaries,

$$\sigma_{ij}n_j = 0, \tag{A.33}$$

the condition on the new transformed boundary is also given by

$$\sigma'_{ij}n'_{j} = 0. \tag{A.34}$$

This statement is proved by direct substitution of the transformation laws. If there are external forces exerted on the boundaries  $F_i$ , then these are, of course, transformed into the forces  $F'_i$ .

# 3. THE HILBERT PROBLEM AND THE INTEGRAL EQUATION OF MUSKHELISHVILI

In treating slit cracks and dislocation pileups in the text, the elegant mathematical theory developed by Muskhelishvili and the Russian school has been invoked.<sup>15</sup> These results will be summarized here. The reader is also referred to an alternative real-variable treatment of some of the same singular integrals by Bilby and Eshelby in the Appendix of their article in "Fracture."<sup>16</sup>

In the fracture problem in Part III, it is desired to find the complex potential function generated from a stress distribution on the crack surfaces. To this end, we write the Cauchy formula for a function  $f_0(z)$  at an arbitrary point not on the cleavage surface in terms of an integral over the contour of Fig. 55:

$$f_{0}(z) = \frac{1}{2\pi i} \int_{L} \frac{f_{0}^{+}(t)}{t-z} dt - \frac{1}{2\pi i} \int_{L} \frac{f_{0}^{-}(t)}{t-z} dt + \frac{1}{2\pi i} \int_{C_{u}} \frac{f_{0}(\zeta)}{\zeta-z} d\zeta.$$
 (A.35)



Fig. 55. Contour for integrals in Eqs. (A.35) and (A.43). The contour encloses the cut L. It contains a pole at z for Eq. (A.35), and circles around  $t_0$  for Eq. (A.43).

Mathematically, the cleavage surface is a branch line, and is denoted by L.  $f_0(z)$  is assumed to be analytic everywhere in the complex plane except on L, and to approach zero at  $\infty$  in such a way that the integral over  $C_{\infty}$  is zero.  $f_0^+$  and  $f_0^-$  are the limiting values of  $f_0(\zeta)$  on the positive and negative sides of L. Hence

$$f_{0}(z) = \frac{1}{2\pi i} \int_{L} \frac{g(t)}{t - z} dt,$$

$$g(t) = f_{0}^{+}(\zeta) - f_{0}^{-}(\zeta).$$
(A.36)

This equation is a solution of a form of the Hilbert problem. That is, it gives f(z) in terms of an integral over a boundary. It should be noted that Eq. (A.31) and other similar results in this Appendix are valid only when f(z) is sufficiently continuous on L, and at its end points.

In the fracture problem, the known stress function on the cleavage plane is not  $f_0^+ - f_0^-$  but  $f_0^+ + f_0^-$ . To proceed in this case, a property of the function

$$\chi(z) = [(z - a)(z + a)]^{-1/2}$$
 (A.37)

is noted. That is, on -a < t < a.

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$$(t)/\chi^{-}(t) = -1.$$
 (A.38)

Hence, the ratio  $f_0(z)/\chi(z)$  has the property

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$$\left[\frac{f_0(z)}{\chi(z)}\right]^+ - \left[\frac{f_0(z)}{\chi(z)}\right]^- = \frac{f_0^+}{\chi^+} - \frac{f_0^-}{\chi^+} \left[\frac{\chi^+}{\chi^-}\right] = \frac{f_0^+ + f_0^-}{\chi^+}.$$
 (A.39)

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Substitution of Eq. (A.39) into (A.36) yields

$$f_0(z) = \frac{\chi(z)}{2\pi i} \int_{\mathbf{L}} \frac{h(t)}{\chi^+(t)(t-z)} dt,$$
  

$$h(t) = f_0^+(t) + f_0^-(t).$$
(A.40)

In this discussion, the function  $\chi$  thus serves the role of an integrating factor, and Eq. (A.40) is a solution of a second form of the Hilbert problem, suitable for application to fracture when the function h is known.

The solutions, Eqs. (A.36) and (A.40), are not the most general functions which can be generated, when g and h are known, because analytic functions can be added to them, which are continuous on the boundary L. Thus, when  $P_a$  is a polynomial of degree n, a more general solution is

$$f(z) = \frac{\chi(z)}{2\pi i} \int_{L} \frac{h(t)}{\chi^{+}(t)(t-z)} dt + \chi(z) P_{n}(z), \qquad h = f^{+} + f^{-}. \quad (A.41)$$

A similar generalization holds for Eq. (A.36). The polynomial is, of course, fixed by the behavior of f at  $\infty$ . Further generalization of Eq. (A.41) can be derived when L consists of multiple segments, not necessarily straight.<sup>15</sup> In the special case of a set of segments lying on the x axis, the integrating factor is simply composed of a product of functions, Eq. (A.37), one for each segment. The results for this latter case have been summarized by Head and Louat,<sup>131</sup> but these more complicated cases will not be required in this article.

The second invocation of the Muskhelishvili theory is in Part VII, where the problem of a pileup of dislocations in the presence of a crack is addressed. In this case, it is desired to invert a singular integral equation similar to those above, a solution which was first given by Muskhelishvili.<sup>152</sup> In this development, the so-called Plemelj equations arise, and we begin with their derivation.

Consider the Cauchy integral

$$\int \frac{f_0(\zeta)}{\zeta - t_0} d\zeta = 0 \tag{A.42}$$

on the contour given in Fig. 55. In this case,  $t_0$  is on the contour L. Then

$$0 = \frac{1}{2\pi i} \oint \frac{f_0(\zeta)}{\zeta - z_0} d\zeta = \frac{P}{2\pi i} \int_{L} \frac{f_0^+(t)}{t - t_0} dt - \frac{P}{2\pi i} \int_{L} \frac{f_0^-(t)}{t - t_0} dt + \frac{1}{2\pi i} \int_{L_1} \frac{f_0^+(\zeta)}{\zeta - t_0} d\zeta + \frac{1}{2\pi i} \int_{L_1} \frac{f_0^-(\zeta)}{\zeta - t_0} d\zeta + \frac{1}{2\pi i} \int_{C_m} \frac{f_0(\zeta)}{\zeta - t_0} d\zeta. \quad (A.43)$$

131 A. K. Head and N. Louat, Aust. J. Phys. 8, 1 (1955).

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<sup>132</sup> N. Muskhelishvili, "Singular Integral Equations." Noordhoff, Groningen, 1953.

*P* (without subscript) denotes the Cauchy principle value, and  $f_0(\infty) = 0$  so that the integration over  $C_{\alpha}$  is zero. Rearranging terms, Eq. (A.43) becomes

$$\frac{P}{\pi i} \int \frac{g(t)}{t - t_0} dt = h(t),$$

$$g = f^+(t) - f^-(t),$$

$$h = f^+(t) + f^-(t).$$
(A.44)

Equations (A.44) are the Plemelj equations,<sup>13</sup> and their inversion is desired for the solution of the dislocation pileup problem. That is, h represents the known external stress on the dislocations, and g represents the dislocation distribution which is sought.

The inversion of Eq. (A.44) is obtained immediately by the application of Eq. (A.41) first to calculate  $f^+(t)$  and then to calculate  $f^-(t)$ . Noting the property, Eq. (A.38), then subtraction of  $f^+(t)$  from  $f^-(t)$ , yields

$$g(t_0) = \frac{\chi^+(t_0)}{\pi i} P \int_{L} \frac{h(t)}{\chi^+(t)(t-t_0)} dt + \chi^+(t_0) P_n(t_0).$$
(A.45)

The polynomial is determined once more by the property of f at  $\infty$ . Again, though there will not be a need for it in this article, when L consists of a set of segments on the x axis, the solution proceeds from an integrating function composed of products of functions like Eq. (A.39), and a general prescription will be found in Head and Louat.<sup>151</sup>

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## CLEAVAGE, DISLOCATION EMISSION, AND SHIELDING FOR CRACKS UNDER GENERAL LOADING

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Abstract-The purpose of this paper is to consider the conditions for the existence of a cleavage crack in a lattice and its response to all types of external loads when shielded by neighboring dislocations. The theory will be constrained to cleavage on one plane and crack branching is not permitted. In the first part of the paper, general relations are derived for the elastic interactions between a cleavage crack and a dislocation and between pairs of dislocations in the presence of the crack. These results are expressed in terms of the local k-field of the crack tip, the shielding contributions from the dislocations, and the complete specification of the forces on the two types of defects. In the second part, criteria for crack cleavage and emission under static conditions are developed for general loading. It is found that for reasons having to do with the basic nature of a crack on the atomic level, that the condition for equilibrium of a cleavage crack involves primarily only the mode I part of the local k field, and that smaller contributions from modes II and III depend on subtle details of the atomic bonding in the crack core. On the other hand, dislocation emission depends on the full specification of all three components of the local k-field. The complete description of the crack tip conditions is then found to be possible in terms of a simple crack stability diagram in the three dimensional local k-space. The primary result is that combined cleavage and emission states are possible under mixed loading wherein a cleavage crack can generate significant plasticity in mode II and III dislocation configurations. In the third part, the overall static equilibrium configuration of the shielded core crack and its dislocation cloud is considered. General theorems developed show that for symmetric dislocation configurations, mode I configurations only shield the k, loading at the crack tip etc. and that the slip force mutually exerted on two symmetrically placed dislocations is exactly zero. Simplified fracture toughness relations are also derived. Finally, the overall picture developed for a shielded cleavage crack under general loading is summarized.

Résumé-Le but de cet article est d'étudier les conditions d'existence d'une fissure de clivage dans un réseau et sa réponse à tous les types de charges externes lorsqu'elle est écrantée par les dislocations voisines. La théorie est limitée au clivage sur un plan et la ramification de la fissure n'est pas permise. Dans la première partie de cet article, nous obtenons des relations génerales pour les interactions élastiques entre une fissure de clivage et une dislocation et entre une paire de dislocations en présence de la fissure. Les résultats sont exprimés en terme du champ-k local à l'extrêmité de la fissure, des contributions à l'écrantage par les dislocations et de la spécification complète des forces sur les deux types de defauts. Dans la seconde partie, nous développons un critère pour le clivage de fissure et l'émission dans des conditions statiques pour une charge générale. Pour des raisons liées à la nature fondamentale de la fissure à l'échelle atomique, la condition d'équilibre d'une fissure de clivage met en jeu essentiellement le mode 1 du champ k local seulement et les contributions plus faibles des modes II et III dépendent de détails subtils de la liaison atomique au coeur de la fissure. Par contre, l'émission de dislocations dépend de la spécification complète des trois composantes du champ & local. On peut alors décrire complétement les conditions à l'extrêmité de la fissure à partir d'un diagramme simple de stabilité de la fissure dans l'espace & local tridimensionnel. Le premier résultat est que des états combinés de clivage et d'émission sont possibles pour des charges mixtes où une fissure de clivage peut produire une plasticité notable dans les modes II et III de configuration des dislocations. Dans la troisième partie, nous considerons la configuration d'équilibre statique globale de la fissure de coeur écrantée et son nuage de dislocations. Des théorèmes généraux que nous développons montrent que pour des configurations de dislocation symétriques, les configurations du mode l'écrantent seulement la charge k, à l'extrémité de la fissure etc. et que la force de glissement exercée mutuellement sur deux dislocations placees symétriquement est exactement nulle. Nous obtenons également des relations d'endurance à la rupture simplifiées. Enfin, nous résumons la situation générale pour une fissure de clivage écrantée dans le cas d'une charge quelconque.

Zmammenfammg-In dieser Arbeit werden die Bedingungen für die Existenz eines Spaltrisses in einem Gitter und dessen Verhalten unter verschiedenen äußeren Lasten für den Fall betrachtet, daß der Riß durch Versetzungen abgeschirmt wird. Die Theorie ist auf Spaltung auf einer Ebene beschränkt, Rißverzweigung ist nicht möglich. Zuerst werden allgemeine Zusammenhänge abgeleitet, die die elastischen Wechselwirkungen zwischen einem Spaltriß und einer Versetzung und die zwischen Versetz-

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ungspaaren in Gegenwart des Risses hetreffen. Die Ergebnisse werden anhand des lokalen k-Feldes der Rißspitze, dem von den Versetzungen herrührenden Abschirmbeitrag und der vollständigen Beschreibung der Kräfte auf die beiden Defektarten dargestellt. Danach werden Kriterien für Spaltrißbildung und ausbreitung unter allgemeinen Lastbedingungen entwickelt. Wegen der im Grunde atomaren Natur eines Risses ergibt sich daß die Bedingung für das Gleichgewicht eines Spaltrisses im wesentlichen nur den Teil der Mode-I des lokalen k-Feldes umfaßt und daß kleinere Beiträge von den Moden II und HI von Feinheiten der atomaren Bindung im Rißkern abhängen. Andererseits hängt die Emission von Versetzungen von der Gesamtheit der drei Beiträge zum lokalen k-Feld ab. Daraus ergibt sich, daß die Bedingungen der Rißspitze mit einem einfachen Diagramm der Rißstabilität im dreidimensionalen lokalen A-Raum beschrieben werden kann. Als wesentliches Ergebnis ergibt sich, daß unter gemischter Belastung eine Kombination von RiB- und Emissionszuständen möglich sind, hei der der Spaltriß zu einer beträchtlichen Plastizität mit Versetzungskonfigurationen der Moden II und III führen können. Des weiteren wird die gesamte statische Gleichgewichtskonfiguration des Risses mit abgeschirmtem Kern und dessen Versetzungswolke behandelt. Entwickelte allgemeine Theoreme zeigen, daß, bei symmetrische Versetzungskonfigurationen, Konfigurationen der Mode I nur die ki-Last an der Rißspitze abschirmen kann, usw. Dabei ist die gegenseitig auf zwei symmetrisch angeordnete Versetzungen ausgeübte Gleitkraft null. Außerdem werden vereinfachte Zusammenhänge für die Bruchzähigkeit abgeleitet. Zuletzt wird das gesamte, für einen abgeschirmten Spaltriß unter allgemeiner Belastung abgeleitete Bild zusammengefaßt,

#### INTRODUCTION

In this paper we develop a general theory of crack shielding by dislocations in the material. The idea is that cracks and dislocations are singularities in the elastic field of the material, and that their collective response to the external applied stress can be addressed in elastic terms. The equilibrium static (and dynamic) configurations are obtained by a balance of forces on each mobile defect, and it will be found that in terms of the force tending to propagate the crack through the material, the other defects generally shield the crack from the external stress. In the language of fracture mechanics, the toughness of the material against crack propagation is due to this shielding.

It is not necessary to apologize for the use of elastic theory in this connection. Since the defects in a material only interact nonelastically when their cores overlap, the elastic approximation is a good one for normal materials, and breaks down in ways that are easy to track, as for example, when dislocation creation, annihilation, and other such defect "reactions" occur. This point of view is, of course, contrary to that adopted in the continuum plasticity theories commonly used in continuum treatments of the plastic field, because we wish to deal here, at least in principle, with the dislocations which are the seat of that plasticity. Theories of this kind have already been proposed and used to treat antiplane strain crack problems by a number of authors [1-7]. In addition, a 2D continuum dislocation shielding theory has been developed by Hart [8], again in anti-plane strain. It is the purpose of this paper to extend and generalize these results into the plane strain case, because of the additional important degrees of freedom and greater realism gained. Sinclair and Thomson [3] have already given some results for the general anisotropic case, and we will extend their work. There is also a close relationship between this work and the "DBCS" crack of Dugdale [9] and Bilby et al. [10], its generalization to plane strain by Vitek [11] and Riedel [12], and the "augmented BCS model" of Chang and Ohr [4, 5].

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Our theory is constrained to the two-dimensional case. Three-dimensional elasticity for interacting dislocations and cracks is intractable except for the simplest configurations, but fortunately considerable insight in many fracture and deformation problems can be gained by remaining in 2D. Thus, the actual 3D configurations will be "smoothed" into 2D. To obtain quantitative results in any particular crystal, anisotropic theory is the mode of choice. However, in anisotropic theory is the mode of specific results, and the more analytic and therefore physical results possible in the isotropic theory are sometimes lost.

The general plan of the paper is to develop the general elastic analysis in the first part, investigate the conditions for cleavage and emission in the second part, and apply the results to crack configurations and toughness relations in the third part.

The principal new physical results obtained here are (1) the stability of a crack against dislocation emission in a material depends upon the local loading conditions as well as the physical parameters. These results are described in terms of a simple crack stability diagram developed in Part II, and (2) the shielding exerted on a crack by dislocations emitted from it exhibits an "orthogonality" property in which different loading modes with their characteristic dislocation configurations do not interact. These results are described in Part III.

#### PART I: GENERAL RELATIONS

#### 1. Elastic potentials in isotropic elasticity

The static elastic field equations are obtained from the combination of the force balance equation

$$\mathcal{F}_{i} = \sigma_{q,i} \tag{1}$$

$$\sigma_{ij} = \lambda u_{ki} \delta_{ij} + \mu (u_{i,j} + u_{j,i}). \quad (2)$$

They take the form

$$(\lambda + \mu)u_{j,\mu} + \mu u_{i,\mu} = \mathcal{F}_{j}$$
 (3)

 $\sigma_{\mu}$  is the stress tensor,  $\lambda$  and  $\mu$  the elastic constants, u, is the displacement field, and  $\mathcal{F}$  is the body force density. In 2D, u, is a function of  $x_1$  and  $x_2$  only. In anti-plane strain,  $u_1 = u_2 = 0$ , and in plane strain,  $u_1 = 0$ . In anti-plane strain, the field equations become the Laplace equation for  $\mathcal{F} = 0$ , and thus  $u_1$  can be written as the imaginary part of an arbitrary analytic function

$$u_{3} = \frac{1}{i\mu} \left[ \eta(z) - \bar{\eta}(z) \right]$$

$$x = x_1 + ix_2$$

and Hooke's law becomes simply

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where

$$\sigma(z) = \sigma_{12}(x_1, x_2) + i\sigma_{11}(x_1, x_2) = 2\eta'(z) \quad (5)$$

where prime denotes differentiation. Likewise, if  $u_1 = 0$ , which defines plane strain, it can be shown [13] that the field equations are satisfied if there exist two independent complex functions,  $\varphi(z)$  and  $\psi(z)$  such that

$$2\mu u(z) = \kappa \varphi(z) - z \overline{\varphi'(z)} - \overline{\psi(z)}$$
(6a)  
$$\sigma_{11}(x_1, x_2) + \sigma_{22}(x_1, x_2) = 2[\varphi'(z) + \overline{\varphi'(z)}]$$
(6b)

$$\sigma_{22}(x_1, x_2) - \sigma_{11}(x_1, x_2) + 2i\sigma_{12}(x_1, x_2)$$

 $= 2[\bar{z}\varphi''(z) + \psi'(z)]$  (6c)

 $u(z) = u_1(x_1, x_2) + iu_2(x_1, x_2)$  $\kappa = 3 - 4\nu$ 

(7) These equations are satisfied everywhere except for regions containing the crack tip and dislocation cores [13, 14], where  $\phi$  and  $\psi$  become nonanalytic. Since we wish to consider distributions of cracks and dislocations explicitly, we shall do so by introducing functions with the appropriate singularities at the and defects. A general solution in 2D is composed of a simple linear combination of anti-plane and plane strain displacements and stresses.

We will consider a single crack situated at the origin, Fig. 1, with its cleavage plane on the negative  $x_i$  axis. Equations for a finite crack are simple



Fig. 1. Coordinate system for crack and dislocation. The crack tip is at the origin with cleavage plane along the negative  $x_1$  axis. The dislocation is at  $\zeta$ . Complex variables are introduced with  $z = x_1 + ix_3$ .

generalizations of those we shall write, but nothing is gained except algebraic complexity from assuming the cleavage plane to be finite, so we assume it extends over the entire negative real axis. The stress boundary condition on this plane is

$$\sigma_{2i}(z) = 0; \quad x_1 < 0.$$

Because of the choice of this geometry, it will prove convenient to replace the third potential function,  $\phi$ , with the function,  $\omega(z)$ , defined by

$$\omega(z) = z \phi' + \psi$$

and the field equations, (6), then take the form

$$2\mu u = \kappa \varphi - (z - \overline{z})\overline{\varphi^{2}} - \overline{\omega}$$
(10a)  

$$\sigma_{11} + \sigma_{22} = 2(\varphi^{2} + \overline{\varphi^{2}})$$
(10b)  

$$\sigma_{22} - i\sigma_{12} = \varphi^{2} + \overline{\omega^{2}} + (z - \overline{z})\overline{\varphi^{2}}.$$
(10c)

The reason for using these modified potentia functions is seen from the third of the equations, where it is noted that on the negative real axis, the laft side of (10c) is zero.

As shown by Rice [15], for a single ended crack, the fields induced by force distributions Fin and F, which are applied to the crack surfaces to create the crack stresses are given by

$$\eta'(z) = \int_{-\infty}^{0} F_{ini}(t) g(t, z) dt$$
  
$$\Psi'(z) = \int_{-\infty}^{0} F(t) g(t, z) dt$$
  
$$g(z) = \frac{i}{2\pi(t-z)} \sqrt{t/z}$$

$$F(t) = F_1(t) + iF_{01}(t)$$
(11)

 $\omega^{*}(z) = \varphi(z)$ (12)

The star operator is defined for any function by

$$\zeta^{\bullet}(z) = \overline{\zeta(\overline{z})} \qquad (13)$$

Thus  $f^*$  is an analytic function of z, while f is not. (It is customary to use the notation f(z) for the star operator introduced here. However, the usage of J can be confused with the complex conjugate f(t), especially when the dependent variable is not indicated explicitly. Hence in this paper, the bar notation will be reserved exclusively for the complex conjugate operator.)  $+F = F_1 + iF_{11}$  and  $+F_{122}$  are applied to the upper surface, and -F and  $-F_{iii}$  to the lower.  $F_{iii}$ is an anti-plane shear stress acting on the cleavage surface generating a traction force in the  $x_1$  direction,  $F_1$  is an open mode tensile stars distribution, and  $F_1$ is an in plane shear stress. They define the traditional modes III, I and II, respectively,

The distributions, F and  $F_{\rm B1}$ , on the crack surfaces are related to the applied stresses at the external boundary of the body, and to stresses induced or the crack surfaces by internal defects by the standard

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argument which says that the induced stresses on the crack surfaces must be cancelled by the F and Fin distributions. The resulting stresses near the tip are K-fields, such that

$$\eta' = \frac{K_{\rm HI}}{2\sqrt{2\pi z}}$$
(14a)  
$$\varphi' = \frac{R}{2\sqrt{2\pi z}}$$
(14b)  
$$K = K_1 + iK_{\rm H}$$
(14c)

with expressions for K which follow immediately from (11) and (12). Again, a general crack stress field is composed of a linear superposition of  $K_{1}$ ,  $K_{1}$  and  $K_{int}$  stress fields, caused by  $F_i$ .  $F_{in}$  and  $F_{int}$  force distributions on the cleavage plane. To avoid problems associated with the infinite crack limit, we will simply assume that the loaded crack has a far field stress field given by [14].

The development to this point is "well known", and serves principally to establish our notation. When a dislocation is present at a point,  $\zeta$ , with Burgers vector  $(b_1, b_2, b_3)$  in the presence of the crack (assumed for the moment to be unloaded and stress free with all F = 0), the potential functions,  $\eta$ , etc. will be composed of the two parts.

$$\eta = \eta_0 + \eta_1$$
  

$$\varphi = \varphi_0 + \varphi_1$$
  

$$\omega = \omega_0 + \omega_1$$

**(15)** 

where  $\eta_0$ , etc. are the potentials for the dislocation in an infinite homogeneous medium, and  $\eta_1$ , etc. are the additional terms which assure that the stress boundary conditions on the cleavage surfaces are satisfied. Thus

$$\begin{array}{c} \operatorname{Re}(\eta') = 0 \\ \varphi' + \overline{\omega'} = 0 \end{array} \right\} x_1 < 0, x_2 = 0.$$
 (16a)  
(16b)

The functions,  $\eta_0$ , etc. can be written from the known dislocation solutions, and are given by

$$\eta_0 = \frac{\mu b_0}{4\pi (z-\zeta)}$$

$$=\frac{2A}{z-\zeta}$$

φá.

$$\nu_{0}' = \frac{2\bar{A}}{z-\zeta} - \frac{2(\zeta-\bar{\zeta})A}{(z-\zeta)^{2}}$$
(17)

$$A = \frac{\mu b_r}{2\pi i(\kappa + 1)}, \quad b_r = b_1 + ib_2 \qquad (17d)$$

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The reader unfamiliar with the form of  $\varphi_n$  and  $\omega_n$  for These integrals are most easily performed in the

with the standard solutions [16]. The second term in (17c) is required by the necessary translational invariance for the dislocation solution in (10a) and (10c).

In the plane strain part of the problem, it appears that the unknown functions,  $\varphi_i$ , and  $\omega_i$ , are independent of one another. However, from the boundary condition, (16b)

$$-(\varphi_0^* + \omega_0^{*'}) = (\varphi_1^* + \overline{\omega_1^*}); \quad x_1 < 0, x_2 = 0.$$
 (18)

In the left side of this equation, both  $\varphi_0$  and  $\omega_0$  are continuous functions on the cleavage plane cut, C, so  $\tilde{\omega} = \omega^*$  on C. Also,  $\varphi_0$ ]<sup>\*</sup> =  $\varphi_0$ ]<sup>\*</sup> and  $\omega_0^*$ ]<sup>\*</sup> =  $\omega_0^*$ ]<sup>\*</sup> for the upper and lower sides of the cut. On the right side,  $\bar{\omega}$  is not an analytic function of z, and is replaced by  $\omega^{\bullet}$ , which is analytic. However, from the definition, (13),  $\bar{\omega}]^* = \omega^*]^-$ . Hence the boundary condition written in terms of  $\omega^*$  takes the more complicated form

$$-\left(\varphi_{0}^{*}+\overline{\omega_{0}^{*}}\right)\right]^{*} = \varphi_{1}^{*}\left[^{*}+\omega_{1}^{*}\right]^{*}$$
$$-\left(\varphi_{0}^{*}+\overline{\omega_{0}^{*}}\right)\right]^{*} = \varphi_{1}^{*}\left[^{*}+\omega_{1}^{*}\right]^{*}. \tag{19}$$

Since the left sides of (19) are continuous functions on C, subtraction gives

> $[\varphi_1' - \omega_1^{*'}]^* = [\varphi_1' - \omega_1^{*'}]^*.$ (20)

This equation shows that  $\varphi_1' - \omega_1^{*'} = \chi(z)$  is a continuous complex function. Since the functions  $\varphi_1$  and  $\omega_1$  were assumed to have no singularities in the entire z-plane outside the cut, C, because they correspond to no new sources of stress,  $\varphi_1' - \omega_1^{\bullet'} = \chi$  is a constant by Liouville's theorem. This constant is taken to be zero, because it is further assumed that no unnecessary stresses at co are added by the functions  $\varphi_1$  and  $\omega_1$ . Hence, except for an irrelevant constant term

$$\varphi_1 = \omega_1^*. \tag{21}$$

Now, the solution for the dislocation-crack fields is immediate. The physical meaning of the boundary condition equation, (16), is that the  $\eta_1$ , etc. terms represent cancelling forces exerted on the boundary equal to the negative of the ne, etc. terms. Hence, from the general Greens function solution, (11), the (17a) result is

(17b)  

$$\eta_{1}'(z) = + \int_{-\infty}^{0} F_{ill}(t)g(t, z) dt$$

$$F_{ill} = -\frac{\mu b_{1}}{4\pi(t-\zeta)} + C.C.$$
(17c)  

$$\varphi_{1}'(z) = + \int_{-\infty}^{0} F(t)g(t-z) dt$$
(17d)  

$$F = -(\varphi_{0}' + \overline{\omega_{0}'}).$$
(22)

dislocations can check the stresses derived from (15) complex t-plane, Fig. 1. When the integrations for #

(8)

(9)

$$\begin{aligned} \eta_{\text{total}} &= \frac{\sigma(z)}{2} = \frac{\mu}{8\pi} \sum_{i} \left\{ \frac{b_{1}(j)}{z - \zeta_{i}} \left( \sqrt{\frac{\zeta_{i}}{z}} + 1 \right) + \frac{b_{1}(j)}{z - \zeta_{i}} \right) & \text{duced in } \mu \text{ etc. a at the crack tip is all three potentia defined by} \\ & \times \left( \sqrt{\frac{\zeta_{i}}{z}} - 1 \right) \right\} + \frac{K_{\text{HI}}}{2\sqrt{2\pi z}} + \eta_{\text{ext}}^{\prime} \quad (23a) & \text{duced in } \mu \text{ etc. a track tip is all three potentia defined by} \\ \varphi_{\text{total}}^{\prime} &= \sum_{i} A_{i} \left\{ \frac{1}{z - \zeta_{i}} \left( \sqrt{\frac{\zeta_{i}}{z}} + 1 \right) + \frac{1}{z - \zeta_{i}} \left( \sqrt{\frac{\zeta_{i}}{z}} - 1 \right) \right\} & \qquad k_{\text{HI}} = \lim_{z \to 0} \left\{ \frac{k_{\text{HI}}}{k = k_{1} + \frac{\sum_{i} \frac{\lambda_{i} (\zeta_{i} - \zeta_{i})}{2(z - \zeta_{i})^{2}} \left[ \sqrt{\frac{\zeta_{i}}{z}} + \sqrt{\frac{z}{\zeta_{i}}} - 2 \right] & \text{then} \\ & + \frac{K}{2\sqrt{2\pi z}} + \varphi_{\text{en}}^{\prime} & (23b) & k_{\text{HI}} = K_{\text{HI}} - \frac{k_{\text{HI}}}{2} \left\{ \frac{b}{\sqrt{\zeta_{i}}} - 2 \right\} \\ & \omega_{\text{total}}^{\prime}(z) = \varphi_{\text{total}}^{\ast}(z) - \varphi_{\text{total}}^{\ast}(z) + \omega_{\text{en}}^{\prime}(z) & (23c) \\ & - \varphi_{i}^{\ast}(z) \times \omega_{i}^{\prime}(z) & (23c) \end{array}$$

where  $\eta_{ext}$ ,  $\varphi_{ext}$ , and  $\omega_{ext}$  are simply the stresses imposed on the uncracked body by remote loading plus "images" of dislocations in external surfaces, plus higher order non K-field terms in the elastic fields of finite cracks.

These equations are written for the *total*  $\eta$ , etc. of **E** collection of dislocations situated at the points  $\zeta_i$  with screw components.  $b_j \approx b_j$ , and edge components,  $b_i(j) = b_i(j) + ib_2(j)$ , because of the linearity of the elastic solutions.

The reader is cautioned about the logical consistency of the equations (23), however, when terms at infinity are included. For example, for a constant stress  $\sigma_x$  at infinity,  $K \to \infty$ . In this paper we are always concerned with K-field dominated problems, where the geometrical effects of crack shape and loading are factored out—that is, in the limit where the product ( $\sigma_x \sqrt{a}$ ) is finite, where *a* is the crack length. Nevertheless, we have included these "hidden" variables,  $\eta_{mi}$ , in (23) because in certain expressions having to do with the force on dislocations, we want to exhibit explicitly the forces which such external stresses have on the dislocations, even though for the crack part of the problem, one has the difficulty alluded to above.

Equation (23a) is already contained in Ref. [3], and (23b) and (23c) are contained in unpublished lecture notes of Rice. These results are in a more tractable form than those of Vitek [11] and Riedel [12], and equivalent to the less explicit results of Hirth and Wagoner [17]. It will prove very useful to retain the fields expressed in terms of the complex potential functions, rather than to attempt to write the far more complicated stress tensor components. Modes I and II are already explicitly generalized as the real and imaginary parts of K, and the anti-plane strain fields, being independent of plane strain, are simply additive to the latter in order to obtain the general two-dimensional result as explained earlier. The dislocation fields above contribute to the K-field of the crack, because of the singularity induced in  $\eta$ , etc. at the crack tip. The local singularity at the crack tip is, however, still of the form  $1/\sqrt{z}$  for all three potentials. If the local k at the crack tip is defined by

$$2\eta'_{\text{total}}\sqrt{2\pi z}$$
 (24a)

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(25)

(26)

$$k = k_1 + ik_{11} = \lim_{z \to 0} \{2\varphi_{\text{terms}}\sqrt{2\pi z}\}$$
 (24b)

$$k_{\rm HI} = K_{\rm HI} - \sum_{j} k_{\rm HI}^{D}(j)$$

$$k_{\rm HI}^{D}(j) = \frac{\mu}{2} \left\{ \frac{b_{i}(j)}{\sqrt{2\pi\zeta_{j}}} + \frac{b_{i}(j)}{\sqrt{2\pi\zeta_{j}}} \right\}$$
(see Ref. [3]), and
$$k = K - \sum k^{D}(j)$$

$$\begin{split} \bar{k}^{p}(j) &= \frac{\mu}{2i(1-v)} \left\{ \frac{b_{i}(j)}{\sqrt{2\pi \zeta_{j}}} + \frac{b_{i}(j)}{\sqrt{2\pi \zeta_{j}}} + \frac{\pi \bar{b}_{i}(j)(\zeta_{i} - \zeta_{i})}{(2\pi \zeta_{i})^{3/2}} \right\} \end{split}$$

where  $K_{iii}$  and K are the far field stress fields of the loaded crack.

According to these equations, the stress singularity at the crack tip is reduced (shielded) by dislocations of positive Burgers vector, and enhanced (antishielded) by dislocations of negative Burgers vector. The stress singularity at the crack tip is characterized by the local stress intensity,  $k_{\rm ill}$  and k, which differs from the long range or macro K-field,  $K_{\rm ill}$  and K. For the semi-infinite crack the long range stress field is still dominated at infinity by the K-field, provided the dislocation distribution is restricted to finite distances. from the crack (small scale yielding approximation). (In this section, for reasons already given, we imagine  $\sigma_{\rm er} = 0.$ )

#### **3.** Forces on 2D defects

In its original 3D form, Eshelby's theorem for the Langrangian force on a defect is [18]

$$f_m = \int (W \delta_{im} - \sigma_{ij} u_{j,m}) \, \mathrm{d}S_i \qquad (27)$$

where  $f_{\rm m}$  is the summed force on a collection of defects enclosed in the surface, W is the elastic energy density function, and S is any surface surrounding the defects. The surface is arbitrary so long as it encloses only the defects in question.

For our purposes, in 2D, this theorem may be written in terms of the potentials,  $\eta$ ,  $\varphi$  and  $\omega$ . After

(28)

direct substitution for the stresses from (6) and (10) dislocation in the crack. The thin the 2D result is b and b(i) where b(i) is the

$$\begin{split} \vec{f} &= \frac{\pi}{\mu} \sum_{nm} [4 \text{Res}\{\eta'^2\} \\ &+ 4(1-\nu) \text{Res}\{\varphi'\omega' - \varphi'^2 - z\varphi'\varphi''\} \\ &+ 2(1-\nu) \overline{\text{Res}}\{\varphi'^2\}] \\ \vec{f} &= f_1 + if_2. \end{split}$$

The integral in (27) becomes in (28) simply a sum over the enclosed residues of the potentials. In this latter equation, the anti-plane and plane strain solutions are explicitly added. According to this equation, the total force on a collection of defects is simply the algebraic sum over the individual defects, as it must be in a linear theory. The reader can verify that the Peach-Koehler force on a single dislocation follows from (28), and that the self force on the dislocation is zero. The anti-plane forms of this equation have been given earlier [3]. These equations are anticipated by the work of Budiansky and Rice [19]. For a different treatment of the force problem, the reader is referred to Chang [20] and to Hirth *et al.* [21]. For a single crack, (28) reduces to

$$F = \frac{1}{2\mu} \left[ k_{111}^2 + (1 - \nu) \left( k\bar{k} + \frac{k^2 - \bar{k}^2}{2} \right) \right]$$
  
=  $k_1 + ik_{11}$ . (29)

The real and imaginary parts of this equation are

$$\operatorname{Re}\{f_{r}\} = \frac{i}{2\mu} [k_{11}^{2} + (1 - \nu)(k_{1}^{2} + k_{11}^{2})]$$
$$I_{m}\{f_{r}\} = -\frac{1 - \nu}{\mu} k_{1} k \bar{u} \qquad (30)$$

The real part is the classic Irwin result (22), while the imaginary part is a force normal to the cleavage plane. Strictly speaking, this is a non-physical motion in which the entire crack, including the cleavage plane, moves in the  $x_2$ -direction. Since a crack is equivalent to a distribution of dislocations on the cleavage plane [23] with an infinite density at the tip, one would imagine that this force is also that for crack branching in the  $x_2$  direction. Unfortunately, direct treatments of the branching problem [24] show that in addition to the term  $k_1k_{11}$ , terms in  $k_1^2$  and  $k_{11}^2$ are also present. The mode III crack experiences no branching force. An important result of (29) is that the force on the crack depends only on the local k at the crack tip.

The force on a dislocation at  $\zeta$  in the presence of a crack and embedded in a cloud of other dislocations at  $\zeta_i$  is considerably more complicated. It is composed of three terms with distinct physical meaning. There is a term bilinear in K and b, which is the direct force by the crack on the dislocation. The sign of this term depends on the sign of the dislocation. A second term is quadratic in b, and is always attractive toward the crack. This term is due to the self image of the

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b and 
$$b(j)$$
, where  $b(j)$  is the Burgers vector of another dislocation in the cloud. Thus

$$f_{d} = f_{Rd} + f_{d1} + \sum_{i} f_{dd_{i}} + f_{mi}.$$
 (31)

In order, the three terms are

$$\begin{split} f[\underline{y}] &= \frac{K_{ul}b_{i}}{\sqrt{2\pi\zeta}} + \frac{1}{2i\sqrt{2\pi\zeta}} \\ &\times \left\{ Kb_{c} - Kb_{c} + \frac{Kb_{c}(\zeta-\overline{\zeta})}{2\zeta} - Kb_{c} \right\} \\ &- \frac{Kb_{c}}{2i\sqrt{2\pi\zeta}} \end{split} \tag{32}$$

$$\begin{aligned} f_{c1} &= -\frac{\mu b_{c}^{2}}{4\pi} \left\{ \frac{1}{2\zeta} + \frac{1}{\zeta-\overline{\zeta}} - \sqrt{\zeta} \frac{1}{\zeta(\overline{\zeta}-\overline{\zeta})} \right\} \\ &- \frac{\mu}{4\pi(1-\nu)} \left\{ \frac{b_{c}^{2}\sqrt{\zeta}}{4\zeta^{5/2}} \left( \sqrt{\zeta} + 1 \right) + \frac{b_{c}b_{c}}{4} \right\} \\ &\times \left[ \frac{3}{\zeta} + \frac{1}{2\sqrt{\zeta}\overline{\zeta}} \left( 1 - \frac{\zeta}{\zeta} \right) + \frac{3 - \sqrt{\zeta}\overline{\zeta}\overline{\zeta}}{\sqrt{\zeta}(\sqrt{\zeta} + \sqrt{\zeta})} \right] \\ &- \frac{b_{c}^{2}}{4\zeta} \left( 1 + \sqrt{\zeta} \right] \right\} \tag{33}$$

$$\begin{aligned} f_{a_{c}} &= \frac{\mu b_{c}b_{c}(f)}{4\pi} \left\{ \frac{1}{\zeta-\zeta_{c}} - \frac{1}{\zeta-\zeta_{c}} + \sqrt{\frac{\zeta}{\zeta}} \frac{1}{\zeta(\overline{\zeta}-\zeta_{c})} \\ &+ \sqrt{\frac{\zeta}{\zeta}} \frac{1}{(\zeta-\zeta_{c})} \right\} + \frac{1}{8\pi(1-\nu)} \\ &\times \left\{ (b_{c}b_{c}(f) + b_{c}b_{c}(f) + b_{c}b_{c}(f) \right\} \\ &\times \left[ \frac{1}{\xi_{c}} \left( \sqrt{\frac{\xi}{\zeta}} + 1 \right) + \frac{1}{\xi_{c}^{2}} \left( \sqrt{\frac{\xi}{\zeta}} - 1 \right) \right] \\ &- b_{c}b_{c}(f) b_{c}iy \left[ \frac{1}{\xi_{c}^{2}} \left( \sqrt{\frac{\xi}{\zeta}} + 1 \right) + \frac{1}{\xi_{c}^{2}} \left( \sqrt{\frac{\xi}{\zeta}} - 1 \right) \right] \\ &- 2b_{c}(f) b_{c}iy \left[ \frac{1}{\xi_{c}^{2}} \left( \sqrt{\frac{\xi}{\zeta}} + 1 \right) + \frac{1}{\xi_{c}^{2}} \left( \sqrt{\frac{\xi}{\zeta}} - 1 \right) \right] \\ &+ \frac{b_{c}b_{c}(f) \mu_{c}}{\xi_{c}^{2}} \left[ \sqrt{\frac{\zeta}{\zeta}} + \sqrt{\frac{\zeta}{\zeta}} + 2 \right] \\ &- \left( \frac{(b_{c}b_{c}(f) + b_{c}b_{c}(f))}{\xi_{c}^{2}} \right) \left[ iy_{c} + 4 \frac{b_{c}b_{c}(f) yy_{c}}{\xi_{c}^{2}} \right] \\ &\times \left[ \sqrt{\frac{\zeta}{\zeta}} + \sqrt{\frac{\zeta}{\zeta}} - 2 \right] - \frac{b_{c}b_{c}(f) yy_{c}}{\xi_{c}^{2}} \left( \sqrt{\frac{\zeta}{\zeta}} - \sqrt{\frac{\xi}{\zeta}} \right) \right\} \\ &\times \left( \frac{\sqrt{\zeta_{c}}}{\zeta_{c}} + \sqrt{\frac{\zeta}{\zeta_{c}}} \right) + \frac{b_{c}b_{c}(f) yy_{c}}{\xi_{c}^{2}} \left( \sqrt{\frac{\zeta}{\zeta}} - \sqrt{\frac{\zeta}{\zeta}} \right) \right\} \end{aligned}$$

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(34)

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$$\ddot{s}_{i} = \ddot{s}_{i} - \ddot{s}_{i}; \quad \ddot{s}_{i}^{*} = \ddot{s}_{i} - \ddot{s}_{i}; \quad y = \frac{v - v}{2i};$$
  
 $y_{i} = \frac{\ddot{s}_{i} - \ddot{s}_{i}}{2i}.$ 

These equations take simple forms for the radial components relative to the crack tip. Physically, this case is important when this direction is contained in a slip plane for the dislocations involved. For this reason we introduce rotated slip plane coordinates. Fig. 2. If the new coordinates are lined up so that the new  $x_1$  is in the slip direction, the new  $x_2$  is in the climb direction, and a is the rotation angle between the original x<sub>1</sub> direction and the slip planes, then for any complex vector. A, its value in the slip plane coordinates is

$$\mathbf{A}^{\mathrm{ap}} = \mathbf{A} \, \mathbf{c}^{-n}. \tag{35}$$

. .

In the slip plane coordinates, the first two force equations taken the form

$$\operatorname{Re}\left\{f_{n,p}^{\operatorname{tar}}\right\} = \frac{K_{\mathrm{tar}}h}{\sqrt{2\pi r}} \cos \alpha/2 + \frac{b_{r}}{2\sqrt{2\pi r}}$$

$$\times \left\{K_{1}\sin\alpha\cos\alpha/2 + K_{\mathrm{tar}}\right\}$$

$$\times \left(2\cos\frac{3\alpha}{2} + \sin\alpha\sin\alpha/2\right)\right\} \quad (36)$$

$$\operatorname{Re}\left\{f_{2}^{\operatorname{tar}}\right\} = \frac{-\mu}{4\pi r}\left[b_{r}^{2} + \frac{b_{r}^{2}}{1-\nu}\right]. \quad (37)$$

These expressions are for the real, or slip part of the force. In these equations, b, is the real edge component for the Burgers vector (i.e. not a complex number), but has an algebraic sign. Hence, the direct crack term  $f_{kd}$  is positive or negative, depending on the sign of the Burgers vector. As it turns out, shielding dislocations are basically attracted to the crack. (For certain angles this relationship is reversed for mode 11 loading.) The image force on the slip plane is always attractive.

#### PART II: EMISSION AND CLEAVAGE CRITERIA

General relations were obtained in the previous sections for forces on cracks and interacting dislocations. The first application of these relations is to the question of the stability of a crack against



Fig. 2. Slip plane coordinates. In slip plane coordinates, the new coordinates are related so the new x1 direction lies along  $r_i$ , and z is the angle of rotation between the original  $x_i$  axis lying on the cleavage plane, and the new



spontaneous dislocation emission. This problem has already been treated for pure mode [ [25], and our

purpose here is to extend the earlier reasoning to the

mixed mode case. The stability of an atomically sharp

crack in the lattice follows from a comparison of the

critical k-field at which a dislocation is emitted from

the crack  $(k_{i})$ , with the critical k-field for cleavage

(k.). These quantities will be derived in turn.

The critical k for emission,  $k_{i}$ , is obtained by calculating the force on an emerging dislocation as a function of its distance from the crack sip, and as a function of k. In this calculation, (31) and (32) are used with K set equal to the local k, and without counting the interactions with other dislocations. under the assumption that they are far from the crack core. When there is not a well defined dislocation free zone near the crack tip wherein the field is characterized by the local k, this calculation breaks down. The force is then given as the sum of (36) and (37). See Fig. 2. Except for special cases of  $k_{\rm H}$  loading when the  $k_{\rm m}$  term in (36) goes negative, the function,  $\operatorname{Re}\{f^{\operatorname{dep}}(r)\}\$ , is shown schematically for  $b_{1} > 0, b_{2} > 0$ in Fig. 3. It will always have a negative range in the elastic limit, and an emerging dislocation will experience a barrier to emission. However, when the cores of crack plus dislocation overlap, the elastic limit breaks down, and (37) is valid only for  $r > r_0$ , where rs is a measure of the collective core size of dislocation plus crack. Emission will thus occur spontaneously for all k > k, where k, is defined as that k for which  $Re{f^{**}} = 0$  and  $r = r_a$  in (37). Thus

 $b_1 k_{11k} f_1(\alpha) + b_2 [k_{1k} f_1(\alpha) + k_{1k} f_2(\alpha)]$ 

$$=\frac{\mu}{2\sqrt{2\pi}r_0}\left(b_s^2+\frac{b_s^2}{1-\nu}\right)$$

 $f_1(\alpha) = \frac{1}{2} \sin \alpha \cos \alpha/2$ 

 $f_2(\alpha) = \cos\frac{3d}{2} + \frac{1}{2}\sin\alpha\sin\alpha/2$  $f_1(\alpha) = \cos \alpha/2$ .

Equation (38) is the emission criterion in mixed loading. The available slip systems and cleavage

(38)



Fig. 3. Elastic force on a dislocation. The force is shown schematically as a function of r. r. is the core radius, and is shown for two possible values, corresponding to stable (brittle) and unstable (ductile) cracks.

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Fig. 4. Emission surface. The surface is the graph of equation (38) which gives the critical values of  $k_1$ ,  $k_{11}$  and  $k_{11}$ for emission of dislocations.

plane fix  $b_1$ ,  $b_2$ , and  $a_2$ ,  $r_0$  in general will depend somewhat on slip and cleavage systems, but will be assumed here to be a material constant. Equation (38) defines a plane in  $(k_1k_{11}k_{11})$ -space as shown in Fig. 4. The intercepts at each axis of  $(k_1k_{11}k_{11})$  space define the critical stress intensity factor for emission in pure loading modes and are denoted by  $k_{\rm b}$ , etc. as given by

$$k_{\mu}^{i} = \frac{\mu b_{r}}{f(\alpha)} \frac{1}{2(1-\nu)\sqrt{2\pi r_{0}}} \quad i = 1, 11$$

$$k_{\rm ML}^{\circ} = \frac{\mu b_{\star}}{f_{\rm j}(\alpha)} \frac{1}{2\sqrt{2\pi r_{\rm e}}}$$

 $k_{\perp}^{\alpha}$  are functions of angle  $\alpha$ . They are shown in

spontaneous emission occurs, while points below the plane correspond to cracks stable against such sponlancous emission. Near the plane, it is possible for thermal fluctuations to overcome the energy barrier for emission, but that possibility is not pursued here. It is an obvious conclusion from equation (38) and Fig. 4 that the appropriate mode 11 loading will lower the k, loading required for emission. Note, of course, that by the same token, because of the algebraic sign of k in (38), that the opposite mode II loading will raise the ku loading required for emission. Similarly, if  $b_i \neq 0$ , the mode III loading will either lower or raise the  $k_1$  loading necessary for emission in the same way, depending on the relative signs of  $b_i$  and  $k_{iii}$ .

#### 2. Cleavage criterion

The second part of the argument concerning crack stability pertains to the criterion for cleavage. Sinclair and Finnis [26] have suggested that an appropriate cleavage criterion would be given by balancing the crack extension force with the surface tension of the opening crack. Thus

$$\frac{1}{2\mu} [k_{11k}^2 + (1 - \nu)(k_{1k}^2 + k_{11k}^2)] = 2\gamma.$$
 (40)

In this equation, we have added the term in  $k_{\rm int}$ , which did not appear in Sinclair and Finnis' condition because of the particular problem under discussion by them. The subscript c relates to the critical value for cleavage, just as the subscript e relates to that for emission.

But equation (40) is patently invalid for one extreme case, and we will argue from this case that (40) Fig. 5. For all values of k above the plane in Fig. 4, is in fact not the appropriate cleavage criterion. Thus,



(39)

Fig. 5. Angular plots for  $k_{b}$ . The intercepts  $k_{b}$ ,  $k_{bc}$ , and  $k_{bb}$  are plotted in (a), (b), and (c), respectively, as functions of the angle, a



Fig. 6. Pure mode III cracking. (a) A cut is made between two rows of atoms denoting the crack, (b) force is applied in mode II. and (c) bonds are allowed to reattach, forming a dislocation.

suppose that  $k_{iii} = k_i = 0$ . Then the construction of Fig. 6 shows that at the critical  $k_{ii}$  for bond breaking by shear, the final result is simply the formation of a dislocation. The reason is that in order to form a crack, some amount of  $k_i$  is required to hold the surfaces of the crack behind the tip open so that rebonding of the surface does not take place. If bonding is allowed, of course, the result is simply dislocation formation. The crucial question then, is, how much  $k_i$  is required?

In order to pursue this question, suppose a crack is loaded in mixed mode I and mode II. Then the elastic force at equilibrium by (40) would be

$$k_{iv}^2 + k_{ikv}^2 = \frac{2\gamma E}{1 - v^2}.$$
 (41)

But, according to Barenblatt [27], if  $k_{le}$  were caused by a (constant) tensile stress equal to the theoretical tensile strength of the solid which operates over a core or "cohesive" distance,  $\delta x$ , and similarly, if  $k_{le}$ were caused by a stress equal to the theoretical shear strength operating over the same core size, then  $k_{le}$  in each case is roughly given by

$$r \sim \frac{2}{\pi} g_i \sqrt{\delta x}.$$
 (42)

Then (41) would read

$$\frac{4}{\pi^2}(g_i^2 + g_j^2)\,\delta x = \frac{2\gamma E}{1 - \gamma^2} \tag{43}$$

where g, in each case refers to the theoretical strength of the solid in tension and shear, respectively. Since g, is always larger than g, [28], the major contribution in (43) is from the mode I loading. The worst case listed in Kelly's review [28] is for NaCl, where the estimated ratio of g, to g, is  $g_i/g_i = 0.65$ , so that the shear mode contribution in (43) is ~40%. In the other cases listed, the shear contribution even for brittle materials is of the order of 10% or less. Nevertheless, the brittle materials where the crack is stable against spontaneous breakdown from dislocation emission are also those where g, approaches

closest to g., and given the qualitative character of these results, and the fact that they invoke subtleties in the cohesive region of the crack tip, the question remains open to more sophisticated atomistic study. It is also conceivable that for cases where the stability of a crack is finely balanced between cleavage and emission, that the  $k_0$  or  $k_m$  contribution to the cleavage criterion could become important. The authors are aware of only one study of the clearage criterion in atomic simulation of a crack under united mode loading [27], and the general results were that  $k_{\rm H}$  loading did not sensibly after the cleavage or terion for small values of  $k_{ik}$ , but that crack branching intervened when significant shear loading was imposed. Since crack branching alters the entire physical picture, our discussion applies only to those cases where branching is not involved. Thus, as an approximation, we will use the simple relation.

$$k_{k}^{2} = \frac{2E\gamma}{1 - r^{2}} \tag{44}$$

as the cleavage criterion. From its derivation, this equation is a necessary elastic opening displacement criterion for the crack, not a bond breaking or true cleavage criterion. The difference between these two criteria is the lattice trapping regime. This simple form for (44) will be reasonably valid for force laws which are smeared out as in a metal, and less valid for highly directed bonds.

#### 3. Crack stability

We are now in a position to write down a complete emission/cleavage criterion by combining equation (44) with (38). This is done in Fig. 7, in terms of



Fig. 7. Crack stability diagram. The intersection of the cleavage surface and the emission surface gives the stability criterion for the crack (emission, line as shown). Ecgion beneath the emission surface and above the cleavage surface is a stable region for the crack. In (b) no intersection occurs in the first occurst.

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which we shall proceed to present the conclusions of and dynamics are allowed, which are beyond the subject of this grant which are beyond the

Figure 7 is to be interpreted in the following way. The cleavage criterion is satisfied "above" the  $k_r$ plane,  $(k_1 > k_k)$ , and the emission criterion is satisfied for k values "above" the  $k_r$  plane. For points above both planes, both emission and cleavage are possible; for points above the  $k_r$  plane but below the  $k_r$  plane, emission but not cleavage is possible; for points above the  $k_r$  plane but below the  $k_r$  plane, cleavage but not emission is possible, and for points below both planes, neither emission nor cleavage is possible. Clearly,  $k_{\rm H}$  and  $k_{\rm H}$  may take negative as well as positive values, after the loading sense is specified, though negative values of  $k_1$  will not have physical sense.

It is important to stress that the specific configuration of the surfaces in Fig. 7 depends on the geometry of the particular slip system envisioned, including the magnitude and sign of the Burgers vector screw and edge components. Since for any assumed cleavage plane and crack line (x1 axis), there are a finite number of allowed slip systems, a diagram must be constructed for each. Normally, of course, due to the crystallography, there is usually considerable symmetry in the problem. We also note that in these plane- and anti-plane problems, dislocations which are skew to the crack line are not encompassed. The fact that such dislocations are observed in most crystals, gives rise to an important limitation to the theory. Such dislocations are nonblunting dislocations, but can give rise to jogs on the crack line and cleavage plane.

There are several physical constraints or conditions which must be combined with Fig. 7 in describing a crack self-consistently. First, as discussed earlier, for a cleavage crack to exist in static equilibrium conditions, it is necessary that the cleavage condition be exactly satisfied. Thus, only points on the k, plane can describe such a crack. Likewise in equilibrium, only points either on or below the emission surface are possible. If a crack exists above the emission surface, then emission occurs until the shielding of the emitted dislocations moves the local k value back onto the emission surface. Points below the emission plane are permitted, of course.

It is important to note that the elastic opening condition, (44), is a necessary condition for the crack to exist, but that the left side of (40) is a true elastic driving force, once the existence of the crack is assured. Thus, when significant components of  $k_{11}$ and/or  $k_{1}$  are present, the minimum driving force possible on the crack can be sufficient to drive it to high dynamic speeds. The condition for overall stability as we have stated it, however, is a static condition, and presumes that conditions have not developed in such a way on the crack that the crack breaks away as a dynamic cleavage event before the emission can intervene. Obviously, events at the crack tip have an unstable quality when time dependence subject of this paper, but which are beyond the subject of this paper, but which will be very important in determining the final behavior of the crack/dislocation system. With this essential qualifying statement in mind, we will pursue the static stability conditions on the crack.

Figure 8 depicts the fate of a cleavage crack which has emitted dislocations in three important categories. In the first, Fig. 8(a), dislocations are emitted in a blunting configuration, i.e. the dislocations have a non-zero edge component,  $b_x \neq 0$ . We shall term these mode I dislocations in an obvious notation. The result of multiple emission of such dislocations is to convert the sharp crack into a wedge. Usually, for simple crystals, symmetric slip planes exist as shown. The angle of the wedge opening is determined by the angle  $\alpha$  between the slip planes and the cleavage plane. If the cleavage plane is also a slip plane, then two additional special cases of dislocation emission are possible, labelled mode II and mode III in Fig. 8. Mode II emission corresponds to emission of edge dislocations, and mode III emission to screw dislocations. The notation in each case is due to the fact that from equation (36) the maximum emission force for mode I dislocations is for an angle  $\alpha > 0$  (at  $\alpha = 0$ the emission force is zero in mode I); while in mode II and III the emission force is at or near a maximum at  $\alpha = 0$ . Mode III is "orthogonal" to modes I and II, and these latter loadings exert no emission force on mode III screw dislocations. A result of considerable importance is that combined mode II and/or mode III emissions do not blunt the crack. That is, the crack remains a fully rigorous cleavage crack after mode II and mode III emission.

Keeping the previous points in mind, we now consider several cases of emission/loading combinations which will illustrate the use of the stability diagram given in Fig. 7.

(a) Consider the mode I emission configurations depicted in Fig. 8(a). We assume that the dislocation



Fig. 8. Dislocation configurations in emission. (a) Mode I, (b) mode II, and (c) mode III.

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has a screw component and an edge component [see equation (38)]. We further assume  $k_{i_1} < k_{i_2}$  so that the k, and k, surfaces intersect in the first octant. Thus, in the region near the  $k_1$  axis, no emission is possible. and the crack remains a pure cleavage crack with no emission. However, with added  $k_{\mu}$  and/or  $k_{\mu\nu}$ , the intersection of k, and k, surfaces occurs on a line labeled the emission line. On this line, emission occurs in the assumed mode I emission configuration. In the negative  $k_{ii}$  or  $k_{iii}$  directions, stability of the crack against emission is enhanced. Normally, as noted earlier. a second slip plane exists at  $-\alpha$ symmetrically placed as in Fig. 8(a). Assuming for example, the f.c.c. case with cleavage on (110), the stability diagram is the mirror image of Fig. 7a in the  $k_1k_{111}$  plane. Thus, in Fig. 7(a), whereas negative  $k_{11}$ and  $k_{\rm HI}$  increase the stability of the crack against emission on the initial system, on the second slip system, negative  $k_{ii}$  will have the opposite effect. The screw dislocation in this system may be either positive or negative, so changing the sign of b thus has the effect of switching the direction of stability relative to km. This analysis for the case considered thus shows that the region around the k, axis possesses a region of stability, but that going away from it in any direction leads to emission on one system or its mirror. Analysis of other crack/slip systems will require a similar reasoning.

(b) Again, in the mode I emission configuration with both b, and  $b_r \neq 0$ , assume that  $k_{k} > k_{w}^{2}$  as shown in Fig. 7(b). In this case, throughout the 1st octant, emission precedes cleavage, and no sharp crack is possible at all in this region. However, emission can be inhibited by negative loading in  $k_{iii}$ or  $k_{ii}$ , and the cleavage crack stabilized. As shown in the previous example, however, usually one has other possibilities—by reversing the sign of  $b_{i}$ , or considering other mode I slip planes—in which emission will be still possible.

(c) Mode II edge dislocation emission. In this configuration, we are by necessity in the mixed loading case, because the cleavage criterion in  $k_1$  must be satisfied. If the dislocations emitted on the cleavage plane are pure edge, then no force is exerted on them by  $k_{11}$  loading, and the stability diagram is two dimensional. Also, there is no force on the dislocation from  $k_1$  because  $\alpha = 0$  in (36). Hence, the stability







Fig. 10. Mixed  $k_i/k_{\mu i}$  loading with emission is mode III at point E.

diagram is the simple construction shown in Fig. 9. Thus, the allowed loadings are shown along the hatched line in Fig. 9, and at the point iE, emission takes place. As noted above, this crack can emit any number of dislocations in the mode II configuration, and still remain a fully brittle cleavage crack.

(d) Mode III screw dislocation emission. As above, the stability diagram is again two dimensional because mode II loading does not put a force on the assumed screw dislocation. The stability diagram so that shown in Fig. 10.

(c) Augmented mode III screw dislogation emission. Suppose again that the crystal is oriented for mode III emission. However, in addition, suppose that mode I emission slip planes also exist. Now the stability diagram becomes complicated by additional emission surfaces. If we assume  $k_u = 0$ , then the stability diagram remains two dimensional, but an additional mode I emission line is imposed. See Fig. 11. Two possibilities are drawn. In ,one, the  $k_u$ , line is below the  $k_c$  line, and no cleavage crack is possible, because blunting takes place in mode I emission before the  $k_c$  line can be reached. However, if the  $k_u$  line, it again possible, and mode III emission can occur.

(f) Augmented mode II emission. In this case, loading in I and II is assumed, with mode:I and mode II slip plane both present. The stability diagram is again two dimensional as shown in Fig. 12. In this



I is permitted as in case (a), then mode I and mode II emission are simultaneously possible at  $E_1$ . In case (b), emission occurs at  $E_2$ .



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Fig. 12. Augmented mode II emission. When loading is mixed mode I and mode II, but emission can occur in mode I and mode II, then two cases are possible depending on  $k_u$ , line. For (a), mode I emission only is possible because  $k_u$ . In eroses the cleavage line at a lower value of  $k_u$ . For (b), mode II emission occurs first along the cleavage line.

case, the  $k_{1k}$  lines is horizontal, because for  $\alpha = 0$ , the contribution to mode II emission force is zero from the  $k_1$  loading. The  $k_1$  emission line is also drawn, and as  $k_{11}$  loading is increased along the  $k_2$  line,  $k_{11}$  emission or  $k_1$  emission will take place first depending on where the relative crossings on the  $k_1$  line take place. Given that only one  $k_1$  emission slip system is possible, then by choosing the sign of  $k_{11}$  or the sign of the mode II Burgers vector property, it will be possible to achieve the  $k_{11}$  emission without triggering the  $k_1$  emission. But, if more than one  $k_1$  emission slip system exists, this may not be possible.

#### PART III: APPLICATIONS TO MODE I AND MIXED MODE LOADINGS

In the previous two parts, the necessary general relations governing dislocation/crack interactions and the criteria for crack cleavage and dislocation emission have been derived. The stage is thus set for applying these results to the overall behavior of crack/dislocation configurations in a material under load. A completely successful theory along this line would lead to material toughness relations, and we will go as far in that direction as simple two dimensional dislocation models can carry us. Needless to say, that will not be very far in direction of a completely deterministic theory, but it will be possible to derive some general and qualitative results which will be useful.

The complete toughness problem consists of solving the force balance equations for the crack and each dislocation self-consistently in order to obtain the

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complete equilibrium configuration of the crackdislocation system. That is, in order for the total force on each defect to be zero, the elastic forces calculated in Part I are balanced by other forces exerted by the lattice. Thus

$$f_c = \frac{k_1^2(1-v^2)}{E} = 2\gamma$$

$$f_{\mu\nu}^{ab} = \sigma_{\mu}b. \tag{45}$$

The first equation is the cleavage criterion of (44). In the second equation,  $\sigma_i$  is the usual friction stress invoked by dislocation modelers, and may, variously, be due to the Peierl's force, forest dislocation, impurity interactions, etc. depending on circumstances.

A many body problem of such magnitude is not tractible, and drastic approximations are necessary to go further. In this paper, we will proceed first to develop the shielding relations for the crack. Some physical insight into the overall problem can in fact be gained from this discussion by itself and without solving the complete equilibrium problem of (45). Then we turn to some general theorems which can be proven for the dislocation cloud, and finally, we present a qualitative toughness argument for the mode 1 crack.

The general character of the formalism developed will allow us to consider the mixed mode case, in which a variety of slip planes are active. A qualitative exploration of the mixed mode situation along the lines begun in Part II will be one of the most interesting results of the paper.

#### 1. Shielding relations for the crack

Equations (24) and (25) for Part I are the basic equations relevant to the ensuing discussion, and will be explored here in some detail. It will be useful to break up the general relations to display their component parts. Thus, from (25) and (26), for each dislocation (suppressing the index *j*) we write for each component of the Burgers vector

$$k_{1}^{p} = k_{11}^{p} \frac{\mu b_{1}}{\sqrt{2\pi r}} + k_{12}^{p} \frac{\mu b_{2}}{\sqrt{2\pi r}}$$

$$k_{11}^{p} = k_{11}^{p} \frac{\mu b_{1}}{\sqrt{2\pi r}} + k_{22}^{p} \frac{\mu b_{2}}{\sqrt{2\pi r}}$$

$$k_{111}^{p} = k_{33}^{p} \frac{\mu b_{3}}{\sqrt{2\pi r}}.$$
(46)

In these equations, r is the distance to the dislocation from the crack tip, and  $\theta$  is the angle measured from the tip. The various coefficients  $k_{\theta}^{D}$  contain the angular dependence of the shielding, according to



We have plotted the four independent angular antishielding when  $\theta > \pi/3$ . The degenerate character dependent terms in Fig. 13 for positive Burgers of the matrix also shows that plane strain and vectors. The sign conventions are such that  $k_{11}^p$ ,  $k_{22}^p$ , and  $k_{11}^{p}$  are shielding contributions for the positive  $b_2$ and small angles,  $\theta$ . That is, the  $k^{\theta}$  contribution in each case is such as to decrease the external loadings.  $K_1$ ,  $K_{11}$ , and  $K_{111}$ , at the crack tip. The curve of Fig. 13(a) shows that  $k_{11}^{p}$  and  $k_{12}^{p}$  changes sign as the dislocation moves from in front of, to behind the crack, i.e. the dislocation changes from shielding to

 $k_{11}^{D} = k_{22}^{D}$ (2) (b) (c) k,

(đ)

Fig. 13. (a) Angular dependence of  $k_{11}^0 = k_{22}^0$  (see equation (46)]. In this and the following polar plots (b-d),  $\theta$  has the range  $0 < \theta < \pi$ . Thus, lobes of the figures extending below the horizontal axis correspond to negative values of  $k^p$  for the corresponding values of  $\theta$ . (b) Angular dependence of  $k_{11}^p$  [see equation (46)]. (c) Angular dependence of  $k_{21}^p$ [see equation (46)]. (d) Angular dependence of kin [see equation (46)].

antiplane strain are "orthogonal" to one another, so that they can be discussed separately.

One of the important applications for these equations will be for dislocations which are emitted from the tip. In this case the  $\theta = \pi$ , and Fig. 8 is relevant. For this case equation (46) becomes

$$t_i^{\rho} = \frac{\mu \sigma_r}{2\sqrt{2\pi r} (1-\nu)} (3 \sin \alpha \cos \alpha/2)$$
 (48a)

$$k_{II}^{\mu} = \frac{1}{2\sqrt{2\pi r} (1 - v)} \times (2 \cos \alpha \cos \pi/2 - \sin \alpha \sin \alpha/2)$$
(48a)

uh

 $b_1 = b_1 \cos \alpha + b_2 \sin \alpha$ 

Figure 14(a) and (b) show the function  $k_1^{\mu}$  and  $k_2^{\mu}$ from (48) as functions of the angle a.

A word is necessary here regarding the functional dependence of (46) and (48) for negative angles,  $\alpha$ . For mode 11 dislocations, where  $b_s = (100)$ , and for screw dislocations with  $b_{a} = (001)$ , the variation in a is as given in the equations. However, for mode [ dislocations, Fig. 8(a) shows that for emitted dislocations that blunt the tip, there is a reversal of the b<sub>1</sub> component of the dislocation for equivalent dislocations at  $\pm \alpha$ . Then in the "slip plane coordinate" expression for b, (48c), equivalent dislocations have reversed Burgers vector; i.e.  $b \to -b$  when  $a \to -a$ . Thus in (48a) and (48b),  $K_1^p$  is overall an even function of  $\alpha$ , and  $k_{\alpha}^{B}$  is an odd function of  $\alpha$  for mode I dislocations! Figure 15 incorporates this effect of sign in (47) and (48).



Fig. 14. (a) Angular dependence of  $k_{\perp}^{\rho}$  [see equation (48)]. (b) Angular dependence of k<sup>D</sup><sub>ii</sub> [see equation (48)]. See also comment on negative lobe in Fig. 13 (a) caption.

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(48c)



Fig. 15. Shielding matrix. See equation (47). The rows correspond to the three modes of shielding, and the columns correspond to the three types of dislocation configuration shown in Fig. 8. The first two columns correspond to asymmetric and symmetric emission in the I configuration, respectively. The (+) sign in the table denotes positive shielding for positive b, and that the shielding is symmetric in the angle,  $\alpha$ . The  $(\pm)$  sign denotes that the shielding is antisymmetric in a, so that symmetric emission yields zero shielding.

In further study of (46), it is important to note that the physical constraint of any crack system is that the crack must satisfy the cleavage criterion (44), and thus it is necessary that  $k_i$  be finite. The various relevant special cases can then be developed as in Part II for mixed loadings of interest. This is done in Fig. 15, in terms of a matrix. The rows of the matrix correspond to  $k^{p}$ , i.e. the rows depict the change in k for each mode of loading due to the dislocation configuration. The dislocation configurations are given by the columns. Two mode I configurations are given, however, corresponding to symmetric and one-sided or asymmetric emission.

The matrix indicates that the off diagonal elements are zero or near zero except in only one case. That is, the dislocation configuration of a given loading mode does not interact with other loading modes (are "orthogonal" in this sense) except for one striking case. The exception is that the asymmetric mode i configuration interacts with the local  $k_{\rm H}$ . The sign of the shielding interaction in that case is such that emission of dislocations asymmetrically in mode I retards additional emission through (46) and (38) so that increasingly higher values of  $k_1$  must be exerted in order to attain the emission condition. Sinclair and Finnis [26] have suggested that through this mechanism, eventually the cleavage condition could be reached, and a brittle transition achieved. Such a transition depends upon asymmetric emission, however, and since the intrinsic conditions at the crack tip would generate an alternating emission on symmetric slip planes, any transition observed depends upon local inhomogeneities in the material which cause an asymmetric loading at the crack tip.

While on this point, we note similar conclusions follow for any screw component of an emitted dislocation in mode I. That is, the screw component by (46) will generate a  $k_{in}^0$  shielding contribution at the crack tip which leads to a reformulated (38) which has the form

$$k_{\rm L}(N) \approx \left| \frac{b_{\rm f}}{b_{\rm f} f_{\rm I}} k_{\rm III}^{\rm B}(N) \right| + C. \tag{49}$$

Here k's are written as functions of N to denote the shielding that takes place, and C is the remaining part of (38) which is not a function of N. (For (49) to be valid, a must be sufficiently in the forward direction ] Again, the critical value of  $k_{\rm L}$  increases with  $N_{\rm c}$ provided all the b, are in the same direction. But, if both signs of b, are possible, which is always the case, then alternating emission of one sign and the next occurs and no net  $k_{ni}$  is generated. If there are inhomogeneities at the crack tip which lift the intrinsic symmetry present, then a brittle transition can again take place. (We note that this argument as well as the one by Sinclair and Finnis has only a rough qualitative validity, because after repeated emission, the shape of the crack is wedge shaped, and the sharp crack results are not valid.)

The striking conclusion (with the one important exception) that the dislocation configuration produced by one mode does not shield or interact with another, what we shall term the "shielding orthogonality", is an important result, and bears on a variety of experimental findings. We shall return to it for a fuller discussion at the end of the paper, where an overall picture derived from shielding theory is compared with the experimental world.

#### 2. Some general theorems

In this section, we prove three general results which can be obtained from elastic analysis for dislocations and cracks. They are important, because the complete crack-dislocation configuration is unsolvable, and thus whenever general theorems can be proved, they are often of great usefulness.

(a) Total force on crack dislocation configuration. The total force on the crack plus its entire dislocation shield can be written in the notation of Part I simply as the sum

$$J_{\text{total}} = J_c + \sum_{i} J_{di}.$$
 (50)

This force is summed not only over each defect in the total configuration, but over the plane and antiplane strain components as well. We will be interested only in the real part of this force, because as explained in Part I, the imaginary part of the force on the crack does not correspond to a physical motion of the crack.

This sum can be computed by a term-by-term sum of the various contributions to the overall force, but there is a more elegant method. It has been pointed out in Part I that the asymptotic forms of the

potentials at  $\infty$  are simple K-fields expressed in terms of the far field parameters, K. Kill. By the residue theorem, this contour integral is the same as if the actual stress field with all the singularities at the dislocations and at the crack were replaced by a simple (mixed) A-field based at the crack tip. The residue from this total effective K-field then from (30) gives the force on the total distribution, as

$$\operatorname{Re}\{f_{\text{total}}\} = \frac{1}{2\mu} \left[K_{\text{till}}^2 + (1-\nu)(K_1^2 + K_{\text{till}}^2)\right].$$
(51)

This expected result is that obtained by the standard J-integral formulation when applied to a continuum plastic field in the small scale yielding limit.

Since the force on the crack itself,  $\vec{L}_{+}$  is given in terms of the local k field there, (26), equation (50) can be written in the form

$$\operatorname{Re}\left\{\sum_{i} f_{i}\right\} = \frac{1}{2\mu} \left\{K_{1\mu}^{2} - k_{1\mu}^{2}\right\}$$

+  $(1-\nu)(K_1^2 - k_1^2 + K_0^2 - k_0^2)$ }. (52)

Another form of this equation is obtained by using the general relation  $k_{10}^0 + k_{10} = K_{01}$ , etc. to obtain

$$Re\left(\sum_{a} f_{a}\right) = \frac{1}{2\mu} \{k_{10}^{a} + 2k_{11}K_{11}^{b} + (1 - \nu)(K_{1}^{b} + 2k_{11}K_{1}^{b} + K_{11}^{b} + K_{11}^{b} + 2k_{11}K_{11}^{b})\}.$$
(53)

These results are entirely rigorous, but they apply to a rather restricted physical situation. That is, the force is the real component, in spite of the fact that in mode I, the slip systems will be at some angle to the cleavage plane, and the real component of the force is partly a climb force. Thus, physically, when the crack moves forward, the rigid motion of the dislocation configuration cannot generally move rigidly with it without a mixed climb-slip motion. For this reason, models have been considered [6] where the slip system is parallel to the cleavage plane so this objection is removed, but we will consider a different strategem here.

Consider the construction first proposed by Sinclair and Thomson [3] shown in Fig. 16. The dislocations in the shield are assumed to have slip planes at some angle  $\pm \alpha$  to the cleavage plane. We presume the crack has achieved a steady static quasi-static motion in which an effective local net Burgers vector is established in the region surrounding the crack. As the crack extends a distance  $\delta x_i$  a self-similar shield is formed at the new crack position,  $x + \delta x$ , by some combination of dislocation motion and generation and a wake of debris is created between the two points x and  $x + \delta x$ . If this debris is proportional to the local Burgers vector density,  $\beta(\underline{x})$ , then the work done in translating the effective distribution  $\beta(x)$  in the element of area dA to the new position is given by

$$\delta W = \sigma_i(\beta)\beta(x) \, \mathrm{d}A \, \delta x \tag{54}$$

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Fig. 16. Moving crack with self-similar shield and wake. For a moving crack, we assume that in steady state, a self-similar shield is generated at each position, and that the snergy of moving this shield is equivalent to creating a wake for each dislocation in the shield

where  $\sigma_i$  is an effective drag stress on the dislocations. In actual practice, this work is primarily performed by heat generation, but dislocation tangles even with a residual net Burgers vector also result. Thus a simulation of the actual dislocation shield can be achieved by postulating a net dislocation Burgers vector distribution on "transport planes" pamilel to the cleavage plane, and with a drag stress  $\sigma_{f}(\beta)$ . The complexity of the deformation problem then is swept up into the function  $\sigma_r$ , and  $\beta$  is presumed to be determined by a self-consistent balance of the forces on the defects as proposed in the introduction of this part in equation (45). In this simulation, it is important that the Burgers vector not be assumed to be parallel to the cleavage plane, so that the motion of the effective distribution is not a pure slip motion, but neither will one be justified in invoking simple climb processes.  $\sigma_i$  in fact covers a multiplicity of such "sins". Only when the dislocation shield is in the pure mode III, or mode II configuration will simple straightforward slip dislocation simulation be justified.

With this physical picture, however, one can make contact with simple fracture mechanics concepts. For example, the elastic force on the dislocation in (52) by the equilibrium postulate in (45) in the continuum limit is

$$\operatorname{Re}\{\mathrm{d}f_{d}\} = \sigma_{f}(\beta)\beta(x)\,\mathrm{d}A. \tag{55}$$

Integrating this expression to obtain the total force on the dislocations

$$\operatorname{Re}\left\{\sum_{d}f_{d}\right\} = \int \beta \sigma_{f}(\beta) \,\mathrm{d}A. \tag{56}$$

If it is meaningful to define a mean value for a (and this possibility depends upon the physics of the deformation process), then (56) can be written amply

$$\operatorname{Re}\left\{\sum_{a}f_{a}\right\}=\sigma_{f}(\alpha)B\quad B=\int\beta\,\mathrm{d}A\qquad(57)$$

(58)

(60)

where B is the total Burgers vector in the shielding cloud. Because of the essentially tensor character of (57), and the other complexities inherent in our definitions of  $\sigma_i$ , we have indicated that it should be considered a function of x. That is to say  $\sigma_i$  in the "climb" orientation when  $\pi = \pi/2$  should be quite different from  $\sigma_i$  in the "slip" orientation,  $\alpha = 0$ . In any deformation field, and for any dislocation

process, total Burgers vector is preserved, when allowance is made for the surface steps where dislocations are annihilated or created at surfaces, or at crack tips. Hence, we have

$$|B| \sin \alpha = COD$$

where COD is the plastic part of the crack opening displacement, and a is defined in Fig. 17.

Combining (58) with (57) and (52), we have the (indirect) images generated by the second dislocation standard fracture mechanics result

$$COD = \frac{\sin \alpha}{2\mu\sigma_i} (K_1^2 - k_1^2)(1 - \nu).$$
 (59)

In this expression, we have not included mixed loadings with  $K_{\rm H}$  and  $K_{\rm H}$  because of the subtleties already described in that case, and because the rather gross averaging envisioned in this simulation will do considerable violence to such detailed questions. o, in (59) is usually taken to be the yield stress, which it is certainly closely related to, but we leave it in this form to emphasize its physical meaning as developed here.

(b) Newton's Third Law for crack and dislocations. The real part of the force exerted by a crack on its dislocation cloud is equal and opposite to that exerted on the crack by the cloud. This theorem follows immediately from (52) when the external K-fields are made zero. That is, since  $K_1 = K_{11} = K_{11} = 0$ , then  $f_{\text{intel}} = 0$  in (51), and

$$\operatorname{Re}\left\{\overline{f}_{r}+\sum_{d}\overline{f}_{d}\right\}=0.$$

In this case  $k = -K^0$  for each mode of loading and  $f_{gp} = 0$ . Thus

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and

$$\operatorname{Re}\{f_{i}^{p}\}_{\substack{\text{composing}\\ (K_{i}^{p})^{2}}}^{\text{composing}} = \frac{1}{2\mu} \left[ (K_{i1}^{p})^{2} + (1 - \nu) ((K_{i}^{p})^{2} + (K_{i1}^{p})^{2}) \right] \quad (61)$$

$$\left\{ \operatorname{Re} \{ \Sigma f_{d} \} \right\}_{\text{instance}} = \operatorname{Re} \left\{ \sum_{d} f_{d} + \sum_{d} f_{dd} \right\}$$
(62)

(c) Interaction force between symmetric dislocations. Consider a symmetric pair of dislocations shown in Fig. 17. We will show that the slip force of interaction between any two such dislocations is zero. That is, when the term  $f_{AF}$ , of equation (34) is written in the slip coordinate system, the component of force on the slip plane is zero. This is a remarkable result, and is not suggested intuitively by inspection of the configuration together with the various types of



Fig. 17. For two-edge dislocations symmetrically placed relative to the cleavage plane, the dislocations-dislocation force component in the slip plane is zero.

in the crack.

For this configuration, the following expressions are valid

. . ..

$$b = b_{r} e^{-n}$$

$$b_{1} = -b_{r} e^{-n}$$

$$\zeta_{1} = \zeta$$

$$\vec{J} = \vec{J}^{dep} e^{-n}.$$
(63)

Then by direct substitution into (34), the result of a tedious algebraic reduction is

$$Re{f_{2}^{u}} = 0.$$
 (64)

This result is also true for two screw dislocations in the same symmetric configuration, shown in Fig. 8(a). [The reader is reminded that (64) refers only to the part of the force on the dislocation at  $\zeta$  which is bilinear in b and  $b_i$ . The self-image term and the direct forces due to the crack and external stresses are, of course, not zero.) This result will be useful when considering symmetrical distributions of dislocations at a crack.

3. Toughness relation for mode 1

Ohr and Chang [4, 5] have augmented the BCS model of a mode III crack [10] by postulating a dislocation free zone at the crack tip. This modification makes it possible to introduce the local k at the tip, which in the BCS model is zero, and then to derive the overall equilibrium crack-dislocation configuration. In doing so, they make the problem one dimensional, because the dislocations are assumed to be distributed in a continuum approximation on the cleavage plane in front of the crack. In mode I, the dislocations must be distributed on a slip plane at an angle to the cleavage plane as in Fig. 8, and the dislocation-dislocation interaction terms, fas, assume the extremely complicated angular dependent form given in (34). Even if only one arm of the dislocation distribution in Fig. 8 is considered at a time, the form of (34) for  $f_{ab}$  is not one dimensional, because of the image-like terms which are generated at the complex conjugate points,  $\zeta_i$ . Thus, the con-

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tinuum analysis developed for the mode III configuration cannot be applied rigorously. The only term in (34) which lends itself to a one-dimensional continuum model is the "free field" term  $1 \cdot (r - r_i)$ , but using an approximation based on this term one is led to a zero dislocation free zone, which does not lead to the mode III limiting condition, and is thus unphysical. Consequently, we have adopted another approach, which does lead to an estimation of the size of the dislocation free zone as well as the deformation zone.

Suppose the crack/dislocation configuration is composed of a super dislocation of strength B on each of the two slip planes emanating from the crack tip and a single (mini) dislocation of strength b, which we identify with the last dislocations emitted from the crack. See Fig. 18. If  $B \gg b$ , then  $R \gg r_i$ , where R and r, are the distances to the super dislocation and minidislocation, respectively. The force balance problem for this configuration can be solved by noting that the for symmetric pairs of dislocations (i.e. mini/mini and super/super) is zero by theorem (64). Further, the positions of the super dislocations will be insensitive to the presence of the mini-dislocations, although not vice versa. If  $\sigma_r$  is the friction stress on each dislocation, then the force balance on a minidislocation is

$$\sigma_{f} = \frac{bK_{1}\sin z\cos z/2}{2\sqrt{2\pi r_{i}}} - \frac{\mu b^{2}}{4\pi(1-v)r_{i}} + f\frac{dv}{d\pi}(R,r_{i}).$$
 (65)

Since  $R \gg r_i$  and  $B \gg b$ , the term  $f^{\text{str}}_{m}(R, r_i)$  can be ysimplified to give

$$f^{\text{dr}}(R, r_{f}) = -\frac{b \sin \alpha \cos \alpha/2}{2\sqrt{2\pi r_{f}}}$$

$$\times \left(\frac{3\mu B \sin \alpha \cos \alpha/2}{(1-\nu)\sqrt{2\pi R}}\right)$$

$$= -\frac{b \sin \alpha \cos \alpha/2}{2\sqrt{2\pi r_{f}}}$$

$$\times \left[K^{D} - \frac{3\mu b \sin \alpha \cos \alpha/2}{(1-\nu)\sqrt{2\pi r_{f}}}\right] \quad (66)$$

where  $K^{D}$  is given by  $k = K - K^{D}$ . We shall drop the subscript denoting mode I loading, but the analysis below only applies to that case.

$$K^{D} = \frac{3\mu B \sin \alpha \cos \alpha/2}{(1-\nu)\sqrt{2\pi R}} + \frac{3\mu b \sin \alpha \cos \alpha/2}{(1-\nu)\sqrt{2\pi r_{f}}}.$$
 (67)

In terms of the local  $k_1$  (65) becomes

$$\sigma_{f} = \frac{k \sin \alpha \cos \alpha/2}{2\sqrt{2\pi r_{f}}} + \frac{\mu h}{4\pi (1-\nu)r_{f}}$$
$$\times (3 \sin^{2} \alpha \cos^{2} \alpha/2 - 1) \approx \frac{k \sin \alpha \cos \alpha/2}{2\sqrt{2\pi r_{f}}}.$$
(68)

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dislocation pair of strength B at distance R and a wini dislocation pair of strength B at distance R and a wini dislocation pair at r, are shown on symmetric slip planes in mode L.

When the local k reaches the critical value for an equilibrium crack, the image term in this expression is negligible when  $\sigma_t/\mu < 10^{-2}$ , as will be assumed. At this point we must relate the super dislocation strength B to  $\sigma_t$  and to K. This can be done by noting that the total net force balance on the two super dislocations is given by

$$\frac{1-v}{2u}(K^D)^2 = 2B\sigma_t \cos \alpha \qquad (67)$$

with the approximation that  $K^{D} \sim K$ 

$$\sigma_f B = \frac{1-\nu}{4\mu\cos x} K^2.$$
 (70)

Equations (70) and (68) are thus two independent equations for  $K_i$  and  $k_i$ , respectively. If we note that  $\sigma_i$  in real crystals should be related to B through a work hardening relation, then (70) and (68) can be combined to yield the desired toughness relation. Thus, we write

$$\sigma_f = \sigma_0 \left(\frac{B}{B_0}\right)^n \tag{71}$$

1.0.

and the final result after the elimination of  $\sigma_f$  and **5** from (71), (70), and (68) becomes

$$\frac{1-\nu}{4\mu\cos\alpha}K_{i_{1}}^{2} = \frac{B_{0}}{\sigma^{1-m}}\left(\frac{k_{1_{1}}\sin\alpha\cos\alpha/2}{2\sqrt{2\pi r_{1}}}\right)^{(1+m+m)}.$$
 (72)

Equation (72) is written for the critical value of an equilibrium crack, with

$$w = \sqrt{\frac{4\mu\gamma}{1-\gamma}}.$$
 (73)

An equation with the same form as this one can be obtained from (57), where  $\sum f_{d} \simeq (1 - v)K_1^2/2\mu$  from (53). (With symmetric dislocation distributions, only  $k_1^p$  contributes.) But the meaning of  $\sigma_i$  in (57) is quite different from the interpretation in (70). In (70) it is assumed that a real dislocation distribution is produced on the slip plane, however, in the reasoning leading up to (57), the dislocations are the "geometrical" residue of a more complicated deformation zone of a moving crack, in which  $\sigma_i$  really describes a more general dissipation process than simple dislocation slip. Thus, both physical configurations are described by the same equation, (72) and (73), but have different meanings in the fracture mechanics sense.

#### 4. GENERAL CONCLUSIONS

In this section, we summarize the overall conclusions of the paper, and apply them to two selected special cases.

(a) A general isotropic elastic analysis of cracks and dislocations under general loading has been developed which includes theorems for the forces on interacting sharp cracks and dislocations, taken either individually or collectively. This analysis is presented primarily in the first part, but the collective response is discussed in Part III. In modes I and II the analytic results display considerable complexity, especially when it comes to writing the dislocationdislocation forces in the presence of the crack. Fortunately, the shielding contributions of the dislocations to the local crack tip singularity are relatively simple, however, and are amenable to separate detailed analysis.

(b) The dislocation emission criterion for a crack is derived for a static crack under mixed loading conditions with results which can be displayed as a planar surface in k-space (i.e. kikinkin space), Fig. 4, termed a crack stability diagram. The emission depends upon the particular slip system considered as well as the loading condition, and a separate emission plane must be drawn for each possible slip system. However, generally it is expected that the slip systems will break down into what we call mode I, mode II, and mode III dislocation configurations shown in Fig. 8. These are the natural dislocation configurations generated by the three pure modes, separately. An important result is that only dislocations in the mode I configuration blunt the crack. A number of special cases were analyzed and will be summarized below.

(c) The cleavage criterion under mixed loading was examined, and to a first approximation, it is found that the cleavage criterion depends only upon the local mode I stress intensity,  $k_1$ . This result differs from a prediction based on a simple balance of forces, but some minor dependence on  $k_{11}$  and  $k_{111}$  can be produced for certain types of force laws. Even these minor effects of  $k_{11}$  and  $k_{111}$  could be important in altering the balance between emission and cleavage when that balance is a very delicate one, but our first order result is that the cleavage criterion depends only on a Griffith condition for  $k_1$ . This cleavage criterion thus plots in k-space as a plane parallel to the  $k_{11}k_{11}$  coordinate plane. (d) Cleavage vs emission for a given slip system is then determined by inspection of the stability diagram in k-space composed of superposing the emission and cleavage surfaces. Emission will occur when the emission surface lies below the cleavage surface, and vice versa. The crack can also branch to a new cleavage system under mixed loadings, but this possibility is not included in the analysis of this paper. Neither are dynamic time dependent effects considered which can also play an important role in the final crack behavior.

(e) Generally speaking, there exists no intrinsically brittle or ductile materials, because if the appropriate slip system exists for a given cleavage plane, emission can be induced by an appropriate loading condition (always provided branching does not intervene). For example, if a crack is stable against emission in pure mode I, and if the emitted dislocation possesses a screw component, then the imposition of sufficient mode III will reverse the stability so that emission is favored, and blunting of the crack will result.

(f) An even more striking prediction is for simultaneous cleavage and emission under mixed loading. That is, suppose the crack is stable in mode I, and then mode II or mode III loading is imposed such that emission occurs on slip systems coincident with the cleavage plane in the material. In this case, the  $k_1$ loading and emission are independent of one another, and the emission does not affect the  $k_1$  at the crack tip. That is, no shielding of  $k_1$  occurs. Conversely, no mode II or mode III "cracking" can occur without sufficient mode 1 at the crack tip to hold the crack open. A number of special case loading/emission configurations are explored in Part II in Figs 9-12.

(g) After dislocations have been emitted in considerable numbers, the results quoted above are modified and extended by the shielding effects of the dislocations. Again, the analysis is simplified by considering only the three simple mode I, II, and III dislocation configurations. The mixed mode loading situations then are summarized in Fig. 15 of Part III, and except for asymmetric emission in the mode I configuration, the shielding is nearly "orthogonal", That is, mode II dislocations shield mainly mode II loading at the crack tip, etc. The analysis of this paper addresses only sharp cracks, of course, and therefore applies only to cases where the crack tip blunting effects can be neglected. Within the sharp crack regime, however, the orthogonality of the shielding leads to rather simple rules for crack behavior. For example, in the mode II configurationin equilibrium, the local k must be located on the cleavage surface in the stability diagram in order for the crack to remain sharp. As  $K_{ij}$  is added, emission in mode II takes place such that the mode II shielding at the crack tip lowers the local stress intensity factor so that the local k is located at the intersection of the mode II emission surface with the cleavage surface. Crack growth takes place when the local k moves above the cleavage plane.

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(h) Under certain limited conditions, the shielding by the emitted dislocations can alter the cleavage/ emission balance at the crack tip. This possibility has already been pointed out for asymmetric emission in the mode I configuration by Sinclair and Finnis [26]. But if emitted mode I dislocations have a screw component, if only one sign of screw is emitted, then crossover from emission to cleavage can again be induced. In both cases, such a result requires that the normal degeneracy which exists at the crack tip be lifted; i.e. either asymmetric emission of edges or emission of only one sign of screw component.

(i) The Ohr Configuration Paradox. Such considerations as in paragraph g above should apply to the thin film crack/dislocation configuration studied by Ohr and coworkers [30]. The configuration is shown in Fig. 19. The slip plane is oriented at an acute angle to the plane of the foil, and the crack is in a mode III emission configuration. But the foil has a mode J stress on the crack as well, and we have argued that this stress must be present to hold open the crack. Ohr and coworkers find that ductile f.c.c. metals as well as some bcc metals exhibit this configuration. The "paradox" consists in the fact that in the f.c.c. metals,  $k_{\rm b} < k_{\rm b}$  is supposed to hold and for the mode 1 emission configuration, we argue that the emission surface always lies below the cleavage surface. The crack-slip plane geometry is shown in Fig. 20(a), where there is found to be only one mode I slip plane which can intersect the crack line in a blunting configuration. But on this slip plane, the crack has a choice of two Burgers vectors, with opposite screw components. A given mode III loading will split the emission surfaces for these two Burgers vectors as shown in the stability diagram in Fig. 21. Emission for one of these dislocations will be inhibited by the mode III loading, while the other will be enhanced. Since in the experiments, extensive mode III emission occurs, it can be presumed that the local k is on the  $k_{\rm m}$  line shown in Fig. 21. (This line is parallel to  $k_1$ because of the independence of anti-plane and plane



Fig. 20. (a) Slip/crack plane configuration for Oha configuration. (b) Emission in mode I (minor component) and mode II (major component).

strain stress states for pure screws.) Since it is believed the intercept of the  $k_{1}$  line on the  $k_{1}$  axis lies below the  $k_{ij}$  intercept for the f.c.c. metals, this crack line cannot be a sharp cleavage crack under the loading conditions which pertain at the tip. Three possibilities exist to explain the observed short equilibrium track which is observed. The first is that the stress conditions in the thin films are not adequately described by the analysis. We believe this is not the case, and that the overall physics is, in fact, described by the two dimensional solutions, though the magnitudes of the stresses are modified. The second possibility is that the proposed simple cleavage criterion is modified by the mixed loading so that the cleavage enterion fails below the emission condition as discussed in Part II. We do not believe that the f.c.c. metals are a likely case where the force laws are sufficiently directional that a strong mixed loading effect would occur for the cleavage criterion. However, this possibility should not be completely ruled out. The third poss-bility,





Emission Lines

Fig. 19. Ohr crack configuration. The foil is pulled in tension, but the crack moves along a slip plane which is oriented at 45 to the direction of tension

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which we favor, is that the crack, in fact, is not sharp. k and the dislocation free zone (also called the inner but has emitted on the mode I plane as well as the mode III plane. If the edge dislocations emitted in mode I are not so numerous as the screw dislocations, but are present so that there is a finite COD at the tip as in Fig. 21, then the crack will remain apparently sharp, but the small  $k_i$  (i.e.  $k_i < k_{i_i}$ ) will be sufficient to hold the crack open even though the Griffith load is not reached. Such a crack, however, will not cleave because  $k_i$  cannot be exceeded quasi-statically because of the intervention of mode I emission. This general picture seems to be confirmed by the fact that when the crack moves into a thicker part of the specimen, mode I emission is observed. This multiple emission case may be a general phenomenon for ductile materials, where shear "cleavage" is observed in a material where no true cleavage should exist. More extensive analysis of the Ohr experiments is indicated, and one obvious problem remaining is that the cleavage condition proposed here needs experimental verification.

(i) Embrittlement of ductile metals-we believe the general results of this paper may have a bearing on the observations that a kind of embrittlement is induced in intrinsically ductile metals wherein a significant but highly localized deformation remains which is localized on the crack plane [31]. If in these metals the local cleavage criterion  $k_k$  is lowered by the standard argument that the intrinsic surface energy is lowered by the external embrittling agent, and if the cleavage plane is also a slip plane, then the arguments of paragraph (g) above could pertain, in which the material shows both the characteristic of a highly brittle material, because cleavage is possible, and also exhibits large amounts of localized plasticity through the mechanism of mode II and/or mode III emission in a mixed mode stress state at the crack tip.

(k) Finally, the analysis has been applied to the problem of toughness in a simplified shielding configuration in plane strain using a super dislocation analysis. This analysis confirms the general findings of the simpler mode III models developed earlier by others, and emphasizes the important role of the local

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elastic enclave) for the overall material response.

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