INTERNATIONAL ATOMIC ENERGY AGENCY
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SPRING COLLEGE IN MATERIALS SCIENCE

ON

"METALLIC MATERIALS"

(11 May - 19 June 1987)

PHYSICAL UNDERSTANDING OF FRACTURE

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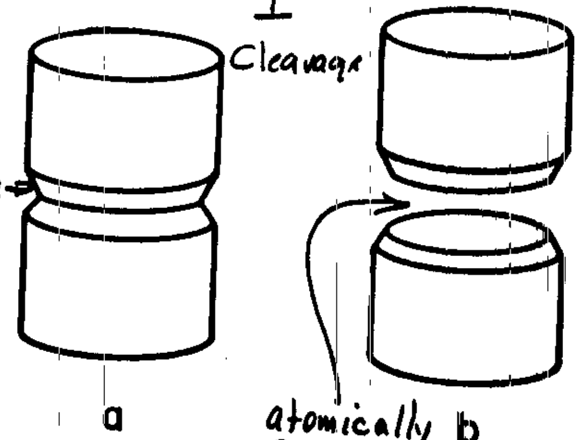
mica
SiO_2 glass
Si
Diamond
etc.

I



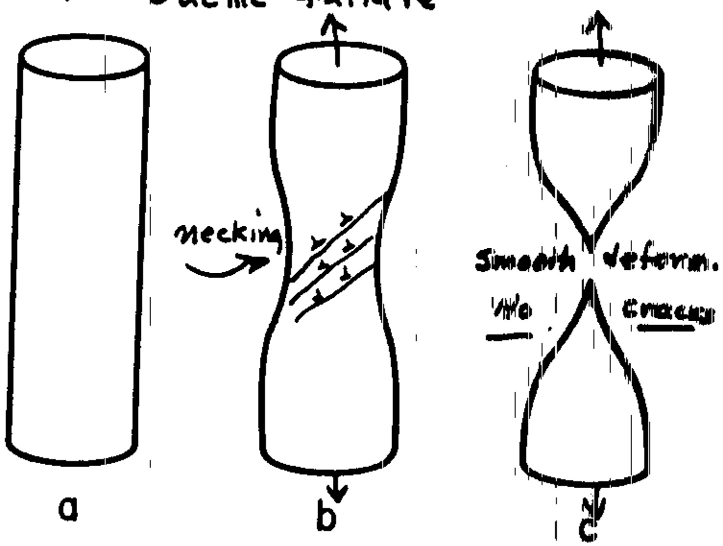
atomically smooth cleavage
(No dislocations or other defect formation)

Failure Bipolarity

II

Ductile failure

"butter"
pure Cu, Al, etc.



Bipolarity

Brittle
High Strength

Si, C, mica
etc.

Ductile
High
Toughness

pure Cu, Au,
Al, etc.

technological materials balanced between high strength + toughness

Balance shifts with:

Strain rate
Temperature
chemical environment
microstructure

Yield – Deformation

Fundamental Problem:

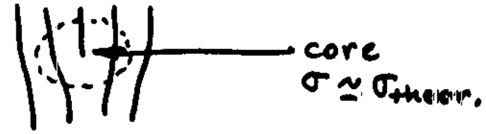
- Why do crystals yield at average stresses much less than bond strength?

Dislocations exist in crystal.

$\sigma \sim \sigma_{theor.}$ in core

translation carries core across entire xtal

translation requires very small σ.



Fracture

Fundamental Problem

- Why do materials crack when average stress is less than bond strenth?

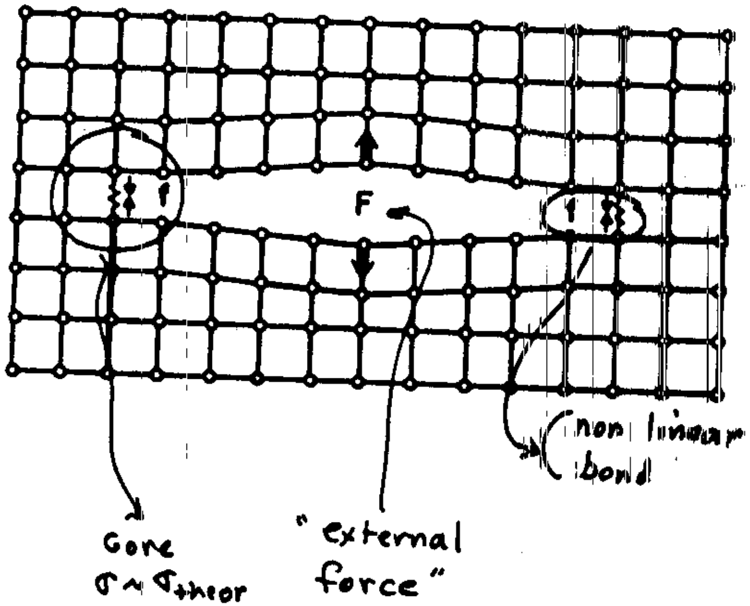
- Cracks exist

$\sigma \sim \sigma_{theor}$ in core

translation carries core across crystal with small external force. result is bifurcation!

Dislocations and cracks are "dual" lattice defects (i.e fundamental lattice defects!) which together determine the ultimate questions of strength and failure of all materials. < what about amorphous matls ?? >

Schematic Model of a Crack



Note: a crack can only exist when an "external" force holds open its cleavage surfaces! (unlike dislocation)

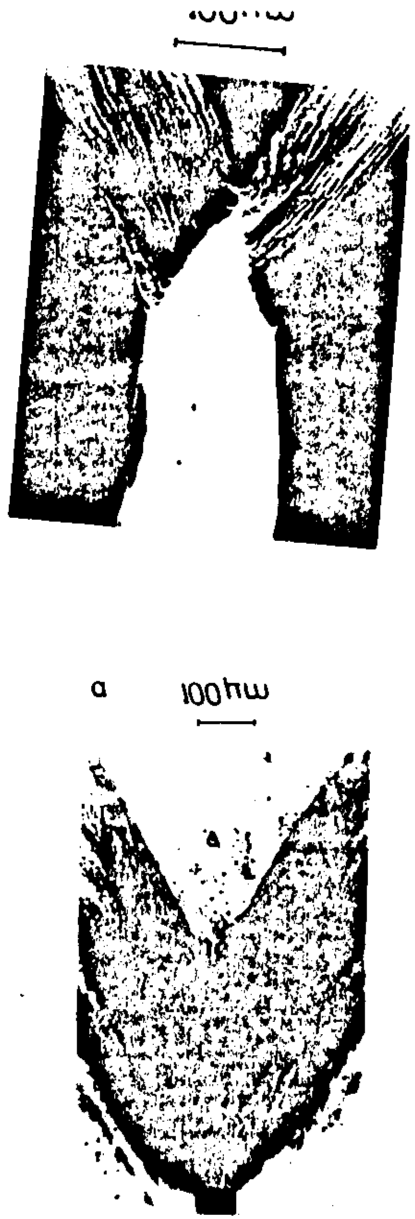
Theoretical Strength of Solids

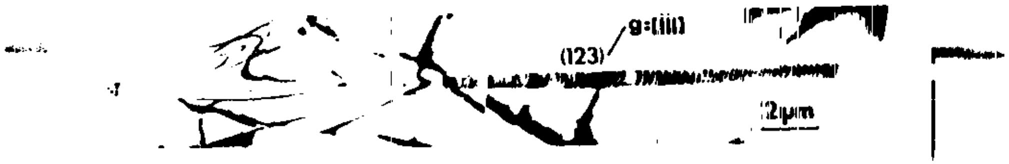
("Strong Solids" by A. Kelly)

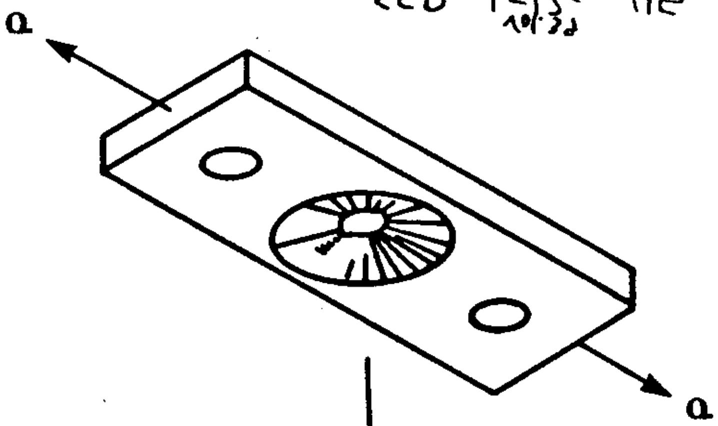
	μ	σ_m (shear)	E	σ_m (tension)	
C	50	12	121	20.[illegible]	
Al_2O_3	15	1.7	46	4.6	
Si	6	1.4	1.0	0.14	
NaCl	2	.3	4.4	0.43	
Cu	3	.13	19.2	3.9	<101>
			6.7	2.5	<100>
Ag	2	.07	12.1	2.4	
Al	2	.09	—	—	
Zn	4	.2	—	—	
Fe	6	.66	26.0	4.6	<111>
			13.2	3.0	<100>

$$\frac{\sigma_{shear}}{\mu} = \left.\begin{matrix} 0.04 & Ag \\ 0.24 & C \end{matrix}\right\} \qquad \frac{\sigma_{tension}}{E} = \begin{matrix} 0.2 & Ag \\ 0.2 & C \end{matrix}$$


1 µm


100 µm
a
100 µm


g=(111)
(123)
2μm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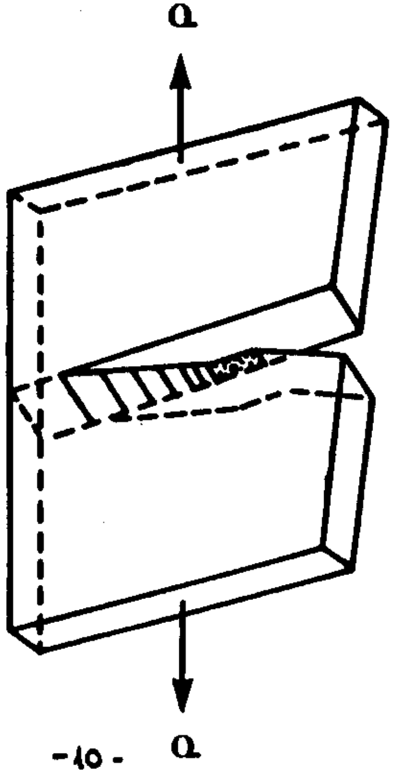
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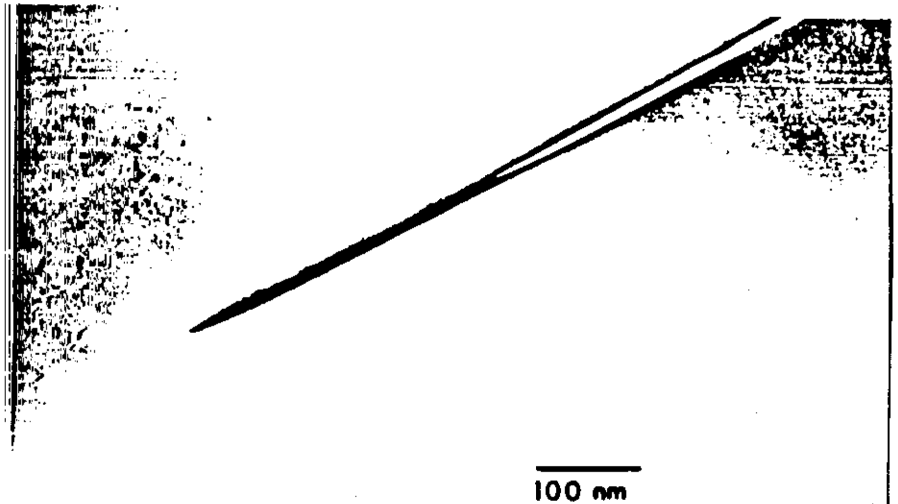
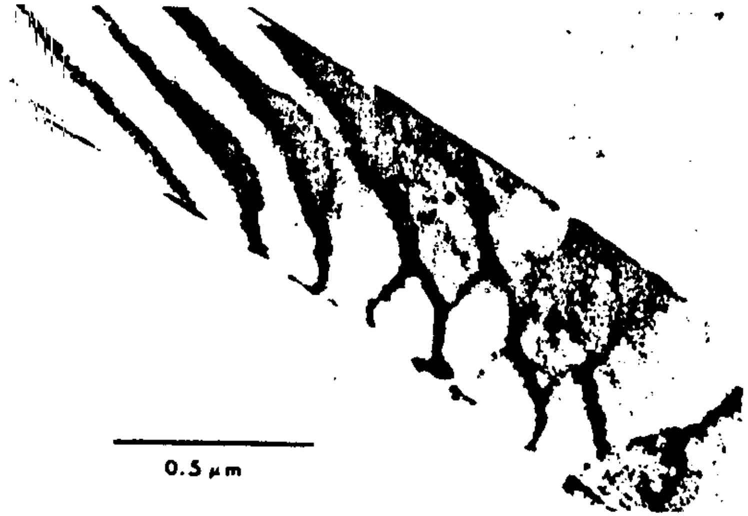
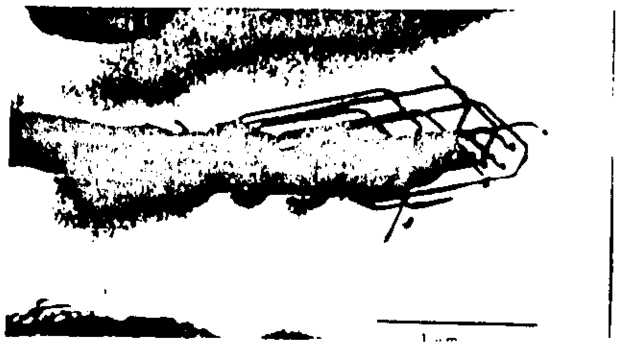

100 nm


0.5 µm



Experimental Background

1. Real failure is <u>very</u> complicated!

2. Modelling done on basis of

   a) 2-D

   b) elasticity (isotropic)

   c) simple atomic lattices

3. Basic Concepts.

   - Interplay between cracks + dislocations
   - Chemical effects on structure of tip
   - Structure of tip determines the ultimate mat'l. behavior

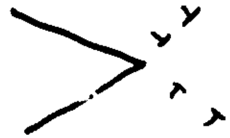
Morpology/Mechanism Relationship

Cleavage

- Bond breaking at Tip (Cleavage Criterion required)
- Dynamic mobility Low toughness
- Shielded by Xlocs.

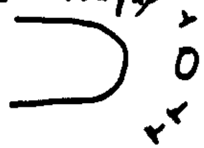
Wedge

- advances by Xloc emission (emission criterion required)
- shielded by Xlocs.
- Hi toughness



Notch

- Blunts - does not advance (hi Tough)
- No singularity at tip
  No emission
  No cleavage
  No shielding
- Absorbs Xlocs from sources
- Fracture by plastic hole growth.



Hints for Theory

1. Interplay between Cracks + Disl. at root of toughness.

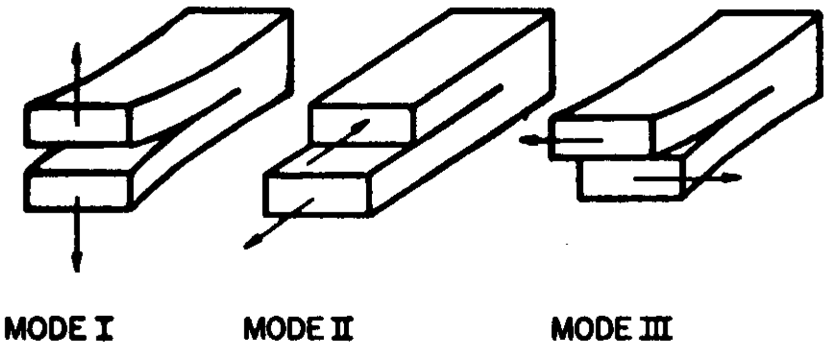
2. A role for chemical interactions with bonds at crack tip.

3. Atomic morphology (structure) of crack crucial. !!

4. Fracture is very complicated
   Simplest modelling is by 2D line defect analysis — (isotropic !)

The Three Primordial Crack "Modes"

(Isotropic medium)



Plane strain (Edge Xloc) (Long. sound waves)

Anti Plane strain (screw Xloc) (shear waves)

2D Elasticity $\left[\frac{\partial}{\partial z} = 0\right]$

See Muskhelishvili
Hirth & Lothe
Rice (Fract. Vol 2)

Stress

force (f) transmitted by ⊕ → ⊖

- $f_i = \sigma_{ij} n_j$ $\quad \sigma_{ij} = \sigma_{ji}$ (no torque)

For equilibrium,

- $\sigma_{ij,j} = f_i$

Linear Response

Strain ⇒ $\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$

Rotation ⇒ $\omega_{ij} = \frac{1}{2}\left(u_{i,j} - u_{j,i}\right)$

$\sigma_{ij} = c_{ijlm}\epsilon_{lm}$

Isotropic

$$\sigma_{ij} = \lambda u_{l,l}\delta_{ij} + \mu\left(u_{i,j} + u_{j,i}\right)$$

surface B.C.

$$\sigma_{ij} n_j = \begin{cases} 0 & \text{Free surf.} \\ F_i & \text{External Force} \end{cases}$$

2D Elasticity

Anti plane Strain

$$u = \begin{Bmatrix} 0 \\ 0 \\ u_z \end{Bmatrix} \qquad \sigma = \begin{pmatrix} 0 & 0 & \sigma_{13} \\ 0 & 0 & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & 0 \end{pmatrix} \qquad \frac{\partial}{\partial z} = 0$$

Equilibrium (no body force)

$\nabla^2 u = 0$ ⇛ Invoke complex variabl $(z = x + iy)$

$\mathrm{Im}\,\eta(z) = \frac{\mu}{2} u$

Hookes Law: $\sigma(z) = \sigma_{32} + i\sigma_{31} = 2\eta'(z)$

$\sigma_{32} = 0$ [B.C]

Functions of class

$\eta(z) = z^n \quad n = \pm\left(\frac{1}{2}, \frac{3}{2} \dots\right)$

$n = +$ → singular at ∞.

$n < 1/2$ → Singular energy in tip region.

$\eta' = \frac{K}{\sqrt{2\pi z}}$ ← stress intensity factor.

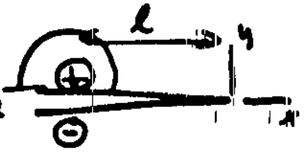
[N.B. $\eta' = \frac{b}{z}$ → Dislocation b real / Line force b imag]

CRACK GREEN'S FN

elegant method — see Appendix SSP.

Heuristic :

Limit $z \to \ell$ must be unit force



$$\lim_{z\to \ell} \int g(z,\ell)_{ij}\, n_j\, d\ell = -1\ \hat{z}$$

$$= \int_0^{\pi} r\left[g_{31}\cos\theta + g_{32}\sin\theta\right] d\theta = -1$$

Thus $g \to \frac{1}{z-\ell}$ at ℓ $\left(f_3 = \mathrm{Re} \oint g\, dz\right)$

Also, must have $1/\sqrt{z}$ at $z \to 0$. to satisfy B.C. on crack surface

Trial: $g = \dfrac{A}{(z-\ell)\sqrt{z}}$

Substitution gives

$$\eta'(z) = g(z) = g_{32} + i\, g_{31}$$

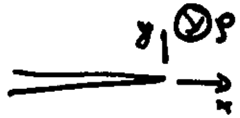
$$g = \frac{1}{2\pi i}\, \frac{1}{(t-z)} \sqrt{\frac{t}{z}} \qquad (t<0)$$

Master Eqn:

$$\eta'(z) = \int_{-\infty}^{0} p(t)\, g(z,t)\, dt$$

p is (Dipole) force distribution on crack surface

Dislocations



In presence of crack,
must add stress (potential) which cancels σ_{yz} on crack surface :

$$\eta' = \eta_0' + \eta_1'$$

$$\eta_0' = \frac{\mu b}{4\pi(z-\xi)}$$

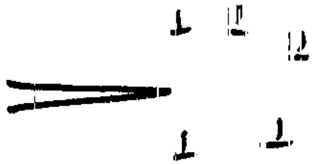
$$\eta_1' = -\frac{1}{2\pi i \sqrt{z}} \int_{-\infty}^{0} \frac{\sqrt{t}\, \mathrm{Re}\{2\eta_0'(t)\}}{t-z}\, dt$$

$$2\eta' = \sigma = \frac{\mu}{4\pi\sqrt{z}}\left(\frac{b}{\sqrt{z}-\sqrt{\xi}} - \underbrace{\frac{b}{\sqrt{z}+\sqrt{\xi}}}_{\text{Image!}}\right) + \underbrace{\frac{K}{\sqrt{2\pi z}}}_{\text{crack}}$$

Many Dislocations : Do summation.

Dislocation Shielding

From Definition of K:



Let k = Local k:

$$k = \lim_{z \to 0} 2\sqrt{2\pi z}\,\eta'$$

From previous page:

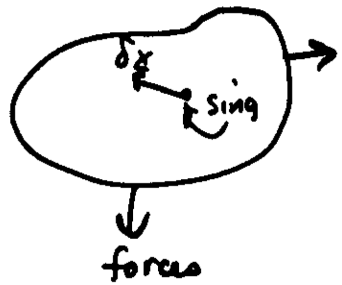
$$k = \underset{\substack{\uparrow \\ \text{external Loading}}}{K} - \underbrace{\frac{\mu}{2} \Sigma\, b_j \left[\frac{1}{\sqrt{2\pi s}} + \frac{1}{\sqrt{2\pi s'}} \right]}_{\text{Dislocation Shielding}}$$

(or antishielding! : $b < 0$)

PRESENCE OF DISLOCATIONS MODIFIES LOCAL CRACK STRENGTH

Eshelby Theorem: Elastic Forces

1. Assume a loaded body containing a singular source of stress.



2. Displace the source δx

Energy density:

$$W = \frac{1}{2} \sigma_{ij} u_{i,j} = W(x)$$

3. Stage 1: calculate change due to translation δx:

$$W^{(1)} = W(x) - \frac{\partial W}{\partial x_k} \delta x_k \quad \text{(Taylor's Th)}$$

(note $-$: due to observer $-$ medium difference)

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

4. Stage 2:

New stresses on body do not satisfy the B.C.!

Eshelby Theorem / con't

New stresses are generated at bndy to assure bndy Cond are satisfied — likewise new displacements also generated., Δu

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

↑ from stage I.

The work done by the stresses working thru these added displacements is:

$$\delta U^{(2)} = \int(\sigma_{ij}+\Delta\sigma_{ij})\,\Delta u_i\, ds_j \simeq \int \sigma_{ij}\,\Delta u_i\, ds_j$$

$$= \int \sigma_{ij}^0\left(u_i^{final} - u_i^{(0)} + \frac{\partial u_i^{(0)}}{\partial x_k}\delta x_k\right) ds_j$$

Stage III : Work Done by external forces:

$$\delta U^{(3)} = -\int \sigma_{ij}^{(0)}\left(u_i^{final} - u_i^{(0)}\right) ds_j$$

Adding:

$$\boxed{f_k = -\frac{\partial U^{total}}{\partial x_k} = \oint \left(W\delta_{ij} - \sigma_{ij}u_{i,k}\right) ds_j}$$

Residue Theorem

In 2-D, replace contour integral by Cauchy theorem:

Mode III $\quad \bar{f} = f_1 + i f_2 = \dfrac{\pi}{\mu}\sum Rs\,(\sigma^2)$

Check for Dislocation:

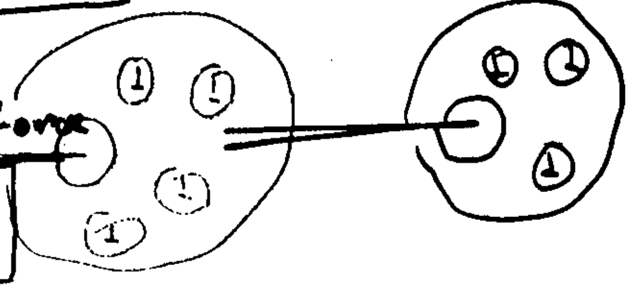
$$\sigma = \sigma_0 + \frac{\mu b}{2\pi z}$$

$$\bar{f} = \sigma_0 b \leftarrow \text{Peach-Koehler}$$

For Crack:

$$\boxed{f_1 = \frac{k^2}{2\mu}}$$

Note (Local stress intensity!)



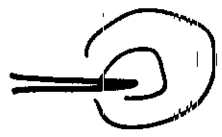
$F = \Sigma f$ = total force

$$\boxed{F = \frac{K^2}{2\mu}}$$

J- Integral

$\Gamma)\quad f_k = \int (W\delta_{ik} - \sigma_{ij} u_{i,k})\, ds = \frac{2\pi^2 i}{\mu}\int \sigma^2 \, d\ldots$

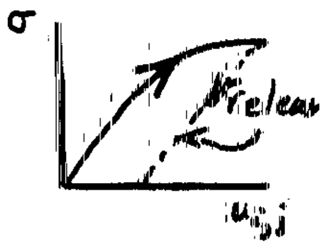
Independent of path by Cauchy theorem



Different Interpretation:

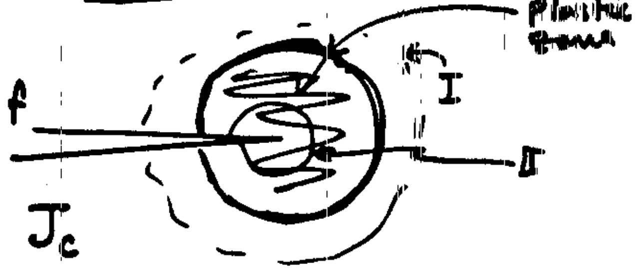
Istead of Hooke's Law,

Let $\sigma = \sigma(u_{i,j})$
(nonlinear)



Then $\boxed{f = J}$ – still independent of path

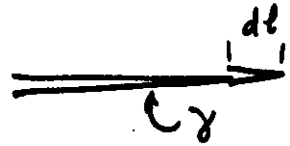
Then J indep. of path, & is a "matl. const". J_c



- characterizes toughness —
- Can Matl "call bluff"?
- great practical use — even fatigue

Griffith Relation

$f_{el} = \frac{k^2}{2\mu}$



$f_{\text{surface tension}} = 2\gamma$

Balance of forces (Conservation of Energy)

$$\boxed{\frac{k^2}{2\mu} = 2\gamma}$$

Based on energy conservation, hence very powerful:

- No disl. activity
- Self similar motion of crack (cleavage)

But γ is a thermodynamic quantity - valid in presence of external chemical environment. So Griffith is a thermo statement, valid under chem. equil. Also limit of kinetics for $v \neq 0$.

Elastic Overview

1. Cracks + Disl. are singularities in El. field

2. $\sigma \simeq K/\sqrt{2\pi r}$ crack

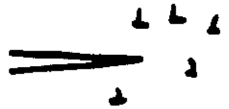
   $\sigma = b/2\pi r$ Disl.

3. Dislocations shield (anti shield) crack.

   k is local field
   K is external field } Note both crack-like!

4. Have developed a formalism for calculating many body equilibrium:

   $$F_{tot} = \Sigma f_{Disl} + \Sigma f_{cracks} = \frac{K^2}{2\mu}$$



   (Large circuit)

5. Each singularity:

   $$f = 0 = f_{elastic} - f_{mat'l.}$$

   γ for crack
   friction stress for X loc.

6. K gives overall toughness — like J — but contains Xloc. effects. (meas. by Narita, et al, Burns, et al)

7. Local Crack equil. given by Griffith — hints at chemical effects.

Limitations

1. Where do Disl. come from?

2. What is shape of crack?

3. Kinetics — (chemical effects) at crack tip?

Overall picture: Toughness is result of dislocation shielding (+ other interplay) with crack.

$\boxed{\text{Toughness is } K_c \text{ at equilibrium.}}$

III ATOMIC AND DISCRETE THEORIES

Atomic treatments do not just remove unsatisfactory singularity –

Required for

Stability of crack in lattice –
(sharp or blunt)

Chemical Effects at tip –
(enhanced reactivity at tip)

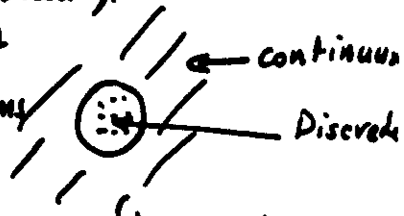
Kinetics of crack motion –
(lattice trapping effects)

Types of Discrete theories

I Classical

1. Inner core with Boundary.

Long history – but flawed by problems on Bndy. 2-D.



[Markworth (Fe, etc.), Mullins, de Cellis, Argon, Yip, (Fe, Cu)

early:

Kanninen et al., Fe

Sinclair Si

2. Pure simulation – Molecular Dynamics

Finite sample, problems of bndy interacting with crack.

Can do dynamic simulations

2-D – so far

Dienes, Paskin, Sieradsky, et al.
(Lennard-Jones)

Doyama

Simmons – ceramics

3. Green's Fns.

∞ Solid, rigorous theoretical base, puts in nonlinearity ad hoc. 3D

II Quantum Theories

All classical theories limited by inadequate force laws.

For metals - used empirical 2-body fit to spline fns. (Johnson Potential) Inadequate for problems where surfaces are present.

For covalents - used empirical 3 body forces (Sinclair: Si)

Ionic Xtals not treated because of long range of force.

Recent progress very dramatic - High promise for powerful theories of detailed crack phenomena:

1. Embedded Atom Method (metals)

Semiempirical method based on embedding potential — metal systems. Used in connection with Molecular dynamics calculations - Fe/H - 3D, still limited to small systems - ~hours on CRAY. Calculations of surfaces, interfaces, dislocations, crack, crack/dislocation. (Kinetics, but not Dynamics)

Daw, Baskes

2. Green's Fns

Small molecular Cluster embedded in a Classical matrix.

Insulators. (Si O)

3-D.

3. Clusters

Molecular calculations of configurations thought to be important in fracture — Interface bonding. (Not a full crack calculation)

Prospect:

First Principle total energy techniques now being applied to surface structure not applied (yet?) to crack.

Crack very complicated extended defect — Prospect is for techniques based on valid first principle concepts to be most successful. Embedded atom good example.

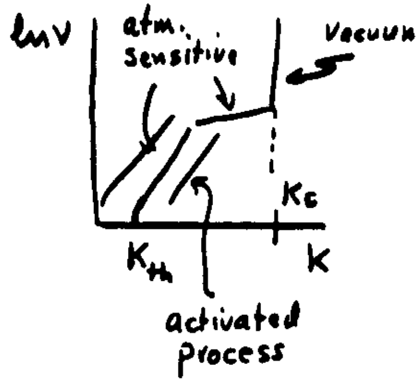
Reaction Paths for Crack Motion

Experimentally (ceramics)

1. In presence of atm., get slow crack growth. growth is activated
2. Occurs in SiO_2, Al_2O_3, MgO, etc.

   (H_2O, etc.)

   (Michalske, Bunker J. Appl. Phys. 56 2686 (1984))



Implication

Some kind of stress induced molecular reaction. Must study local fluctuations (SD) in crack config. induced by chemical reactions at local site.

a) Small molecules: Reaction at tip bond.

b) Large molecule: Penetration into crack mouth restricted.

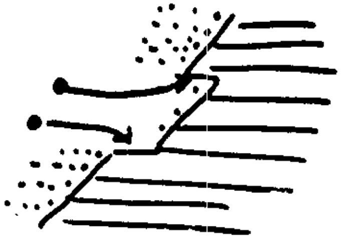
- What is criterion for penetration?
- What mechanisms exist for growth for no penetration?

Plan of Attack

1. Small molecules: penetration assured.

   Assume molecule attacks crack tip bond.

   After reaction, surface is covered $\gamma_0 \rightarrow \gamma_1$ in Griffith relation

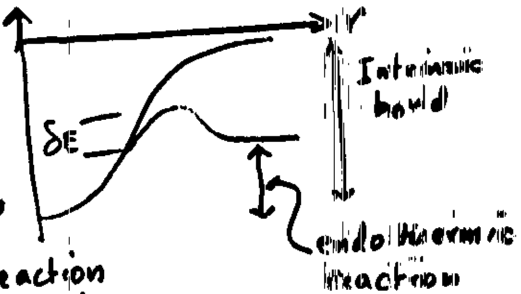


Crack growth is by nucleation & growth of kink pairs on crack tip.

How do barriers arise??

1. Atomicity: Lattice trapping
2. chemical reaction barrier

Bond energy diagram



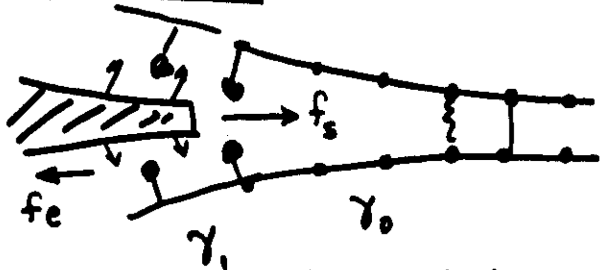
δE = reaction barrier.

Plan of Attack (cont)

2. Large Molecules.

Penetration criterion

Molecular wedge



Elastic force on wedge tip $= f_e(R)$ due to crack surfaces "squirting" molecules out of crack mouth

Surface tension force on wedge tip $= f_s$

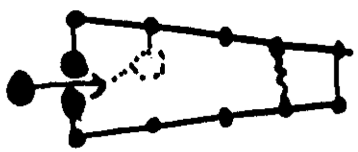
$$f_s = 2(\gamma_0 - \gamma_1)$$

$$\boxed{f_e = f_s \quad \text{at equilibrium}}$$

Penetration condition — depends on R, x.

Mechanism for Crack Growth

Diffusion of molecules in constricted region



Reaction Paths for Small Molecules

(In both cases) Atomic structure of crack is crucial.

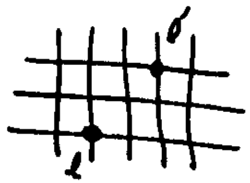
Thus require general theory of crack structure required:

Paradigm

1. Develop a Green's fn. formalism for <u>linear</u> cracked lattice
2. Put in non linear bonds.
3. Calculate reaction path, + $E_{act.}$ (kinked crack)
4. Include external chemical species
5. Entire procedure assumes knowledge of force laws.

Green's Fns Analysis

static Eq'm:



$$\sum_{j,\ell'} \varphi_{ij}(\underline{\ell},\underline{\ell}')\, u_j(\underline{\ell}') = F_i(\underline{\ell})$$

$$\underset{\sim}{\Phi}\,\underline{u} = \underline{F}$$

See Tewary, Adv. Phys. 47 486 (1976)

G defined by

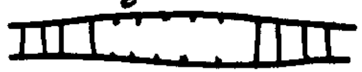
$$G = \Phi^{-1}$$

$$u = GF \qquad \text{("Master" Eqn)}$$

If lattice is defective, then,

$$\Phi^* = \Phi - \delta\Phi \;;\; u = G^*F$$

$\delta\varphi$ (broken bonds)



If

$$G^* = (\Phi^*)^{-1} \quad \text{i.e. } G^*\Phi^* u = G^* 1$$

$$G\left[\Phi - \delta\Phi\right]u = G\cdot 1 \qquad ;\; u = G^*\cdot 1$$

$$\boxed{G^* = G + G\,\delta\Phi\, G^*} \qquad \text{Dyson Eqn.}$$

Formal soln of crack problem. (Note G^* on right)

Assumptions

$u = u_y$

$$f(\ell) = \overset{\text{shear}}{A}\left(\Delta_x^2 + \Delta_z^2\right)u(\ell) + \overset{\text{stretch}}{B}\left(\Delta_y^2\, u(\ell)\right)$$

(nearest neighbor forces)

Then Fourier analyze f, and $G(q)$ is simple:

$$G(q) = \frac{1}{4\left(A\sin^2 q_x/2 + A\sin^2 q_z/2 + B\sin^2 q_y/2\right)}$$

Ultimately, (see notes) Dyson eqn. becomes:

$$\sum_{\substack{\text{crack}\\ \text{plane}}} \left(\delta_{\vec{\ell},\vec{n}} - \alpha(\vec{\ell}-\vec{n})\right) G^*(\vec{n};\vec{m}) = \frac{1}{2B}\,\alpha(\vec{\ell}-\vec{m})$$

$$\alpha(\vec{\ell}-\vec{n}) = -\frac{iB}{8\pi^2 L_z}\sum_{q_z}\int_{-\pi}^{\pi} d\vec{q}\, \frac{e^{i\vec{q}(\vec{\ell}-\vec{n})}\, e^{iq_y\ell_y}\sin q_y/2}{A\left(\sin^2 q_x/2 + \sin^2 q_z/2\right) + B\sin^2 q_y/2}$$

Only integration is analytic.

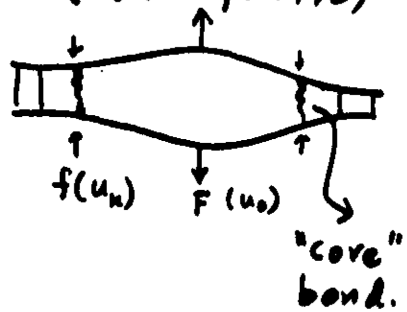
Structure of Eqn:

1. set of algebraic eqns.
   rank of matrix $= N =$ no. atoms on crack basic cell.
2. If $u = (u_x, u_y, u_z)$, and forces are longer range,
   rank $= 3qN$ $\quad q$ = range of force.

Non Linear Bonding Paradigm

(Esterling, 1976)

Green's fn. Master Eqn.:



$$u_0 = g_{00}F - \Sigma g_{0k} f$$
$$\simeq g_{00}F - p\, g_{0k} f$$

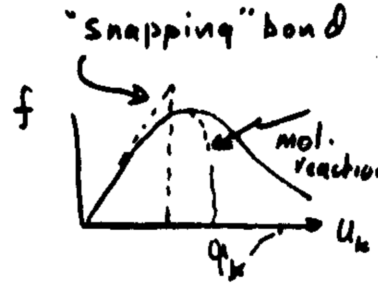
$$u_k = g_{k0}F - \Sigma g_{kk'} f$$
$$= g_{k0}F - g_{kT} f$$

$$\left(u_{k+1} = g_{k+1,0}F - \Sigma g_{k+1,k'} f\right)$$

In the Green's fn. eqn., f is considered an **External** force.

Actually

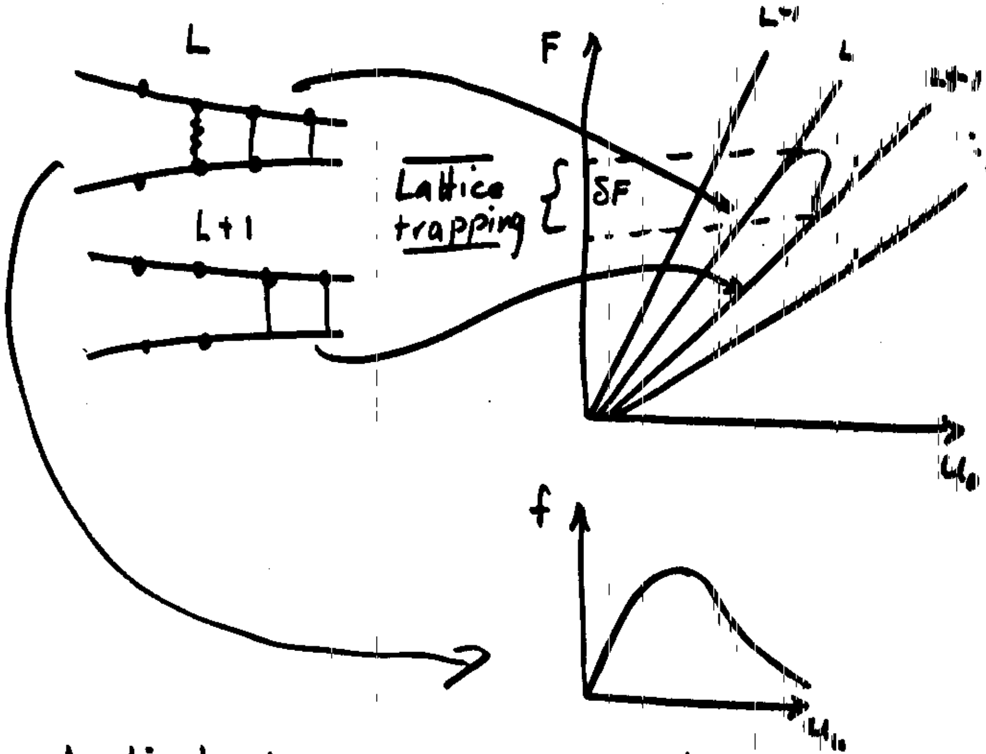
$$f = f(u_k)$$



Thus, the actual crack structure problem is represented by a **Small set** of non linear coupled equations where $N =$ (no. nonlinear bonds) $+ 1$

This represents the real power of Green's fn. Analysis!

Crack Response Fns + Graphical Analysis



As tip bond goes nonlinear + breaks, response fn. goes from $L \to L+1$, with nonlinear excursion between $F(u_0)$ lines.

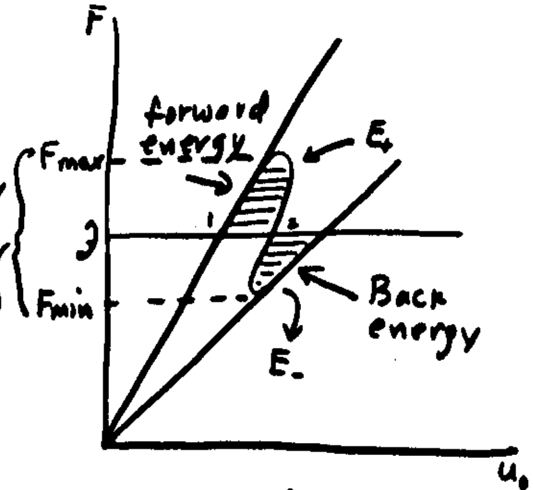
Over lattice trapping range, crack does not change length. This results in energy barriers.

Energy Barriers

$$\Delta E = \int_1^2 F\,du_0 - \mathcal{F}\Delta u_0$$

(internal energy) (work done by external machines.)

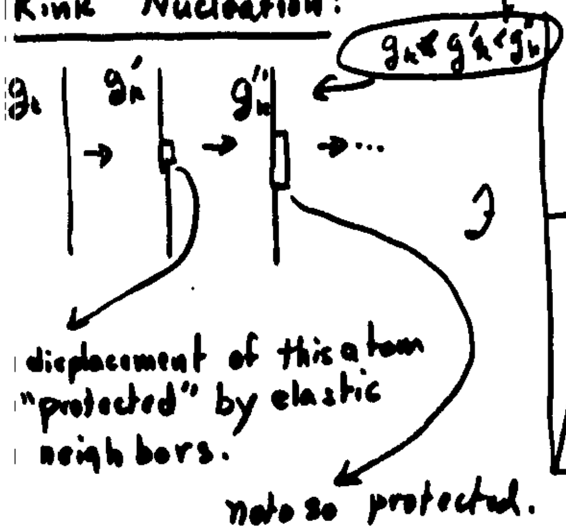
trapping range (mechanical stable)

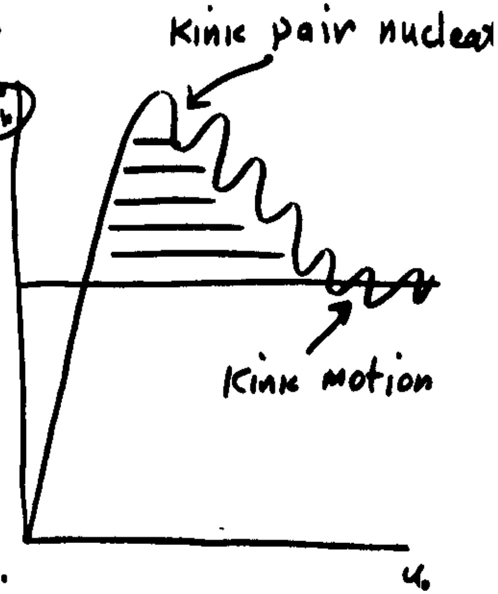


$\mathcal{F}_{Griffith}$: $E_+ \simeq E_-$

valid for kink motion energy, or for 2D crack motion.

Kink Nucleation:





-cont-

1). $E(f(u))$ (very sensitive)

2) Master Eqn $\longrightarrow$ $F(u_o)$ $\longrightarrow$ E

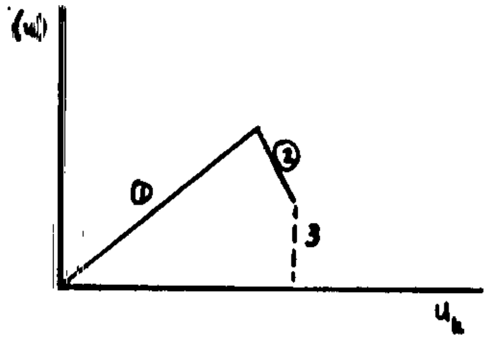
3) $E \to 0$ as core size increases.

[as atomic "size" decreases, uniform elasticity takes over. $\therefore E \to 0$]

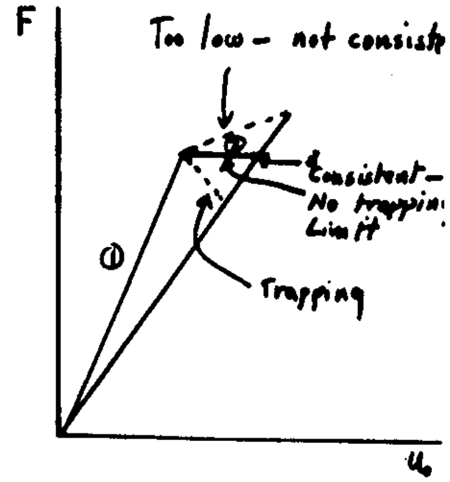
"One Atom" core has most pronounced barriers.

In this case, Master Eqn. degenerates to just $\underline{\underline{2}}$ eqns.

One Atom Core Criterion



Self consistent force Law for limiting response function.



Limiting response curve for zero trapping and self consistent 1 atom core.

From, Green's fns Master Eqn.

$$du_k = g_{ko}\,dF - g_{kr}\,df \qquad (dF = 0)$$

$$\boxed{\left[\frac{df}{du_k}\right]_{\text{lower side}} < -\frac{1}{g_{kr}} = -\frac{B}{h_{kr}}}$$

← elastic modulus

← number (dimensionless)

For trapping to be observable, force law must be almost snapping. Thus, no trapping for intrinsic fracture, external atm. required – special reaction

Green's Fns Summary

- Excellent method for exploring barriers to crack growth with external chemical environment
- Important to develop criterion for penetrati
- Crack growth by chemical reaction at tip only possible for reaction paths of "snapping" character.
- Kink formation energies in SiO_2 ≈ 2 eV motion energy ~ 0.1 ev.
- Qm calculations of forces for insulating matls relevant + needed.
- Diffusion mechanism for barriers still not worked out.

DISLOCATION EMISSION

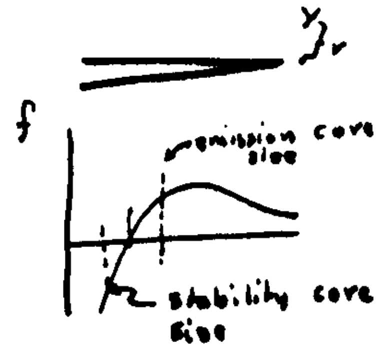
Issue here is Ductile/Brittle dichotomy.

Criterion explored first in elastic cut-off:

2D

In Mode I, (see L+T, Eqn 36)

$$f\Big]_{\text{slip}} = \underset{\substack{\uparrow \\ \text{k-field}}}{\frac{k\,b}{\sqrt{2\pi r}}\,f(\theta)} - \underset{\substack{\uparrow \\ \text{Image}}}{\frac{\mu b^2}{4\pi r(1-\nu)}}$$



when $r = r_{core}$, then emission just possible. Thus:

$$k_e = \frac{\mu b}{2\sqrt{2\pi r_0}\,(1-\nu)}\,\frac{1}{f(\theta)}$$

But Cleavage will occur when

$$k_c = 2\sqrt{\mu\gamma(1-\nu)}$$

Thus

$$\boxed{\begin{array}{l} k_c < k_e \longrightarrow \text{cleaving Crack} \\ k_c > k_e \longrightarrow \text{emitting Crack} \end{array}}$$

A curious parameter:

$$\frac{k_e}{k_c} = \sqrt{\frac{\mu b}{\gamma}} \times \text{const.}$$

Thus

$\frac{\mu b}{\gamma}$ is a figure of merit (rough)

$\frac{\mu b}{\gamma} > 10$ – brittle

$\frac{\mu b}{\gamma} < 10$ – ductile

Roughly the fcc metals are ductile, ionics + [illegible]. brittle. Fe borderline!

But this criterion contains r_o and τ – which are force law parameters.

The real conclusion is that ductile/[illegible] solid depends sensitively on the force laws of solid!

Hence the true emission/cleavage criterion should be done from fundamental theory!

Simulation work –

1. Dienes et al.: confirmed that cut-off criterion is valid for Lennard-Jones 6/12.

2. [redacted] de Celis, Argon, Yip.
   Comp. sim. calc using empirical "Johnson" type force laws. suggest Cu ductile + Fe brittle. – not based on adequate force laws.

3. Daw + Baskes
   confirm Fe is border line – curious result that H enhances Xloc. emission!?

Effect of Mixed Mode

Emission Criterion

Same as before: calculate elastic force on dislocation:

$$f_e = b_s k_{III} f_3(\theta) + b_e \left[k_I f_1(\theta) + k_{II} f_2(\theta) \right]$$

compl. fn. of θ. (see L+T)

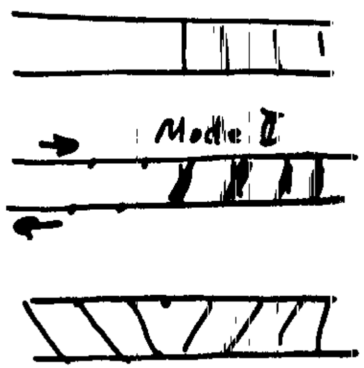
$$- \frac{\mu}{2\sqrt{2\pi r_0}} \left(b_s^2 + \frac{b_e^2}{1-\nu} \right) = 0 \quad \text{for critical pt.}$$

Cleavage Criterion

cut. ①

stress ②

release bonds ③



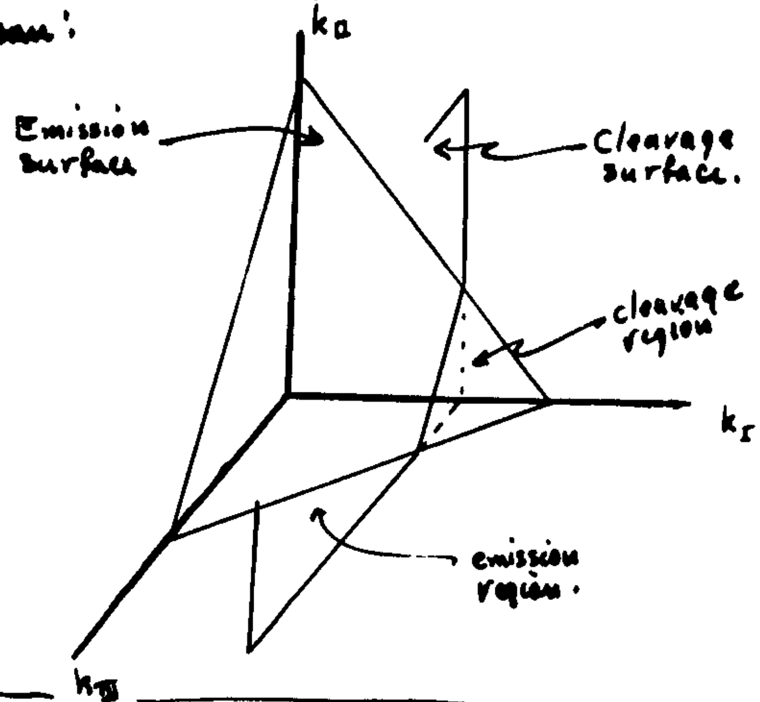
—

Result is a dislocation! Must have sufficient Mode I to open crack on back side of disl. core so crack does not reclose.

I estimate the modification of Griffith relation by Modes II & III to depend somewhat on type of bonding (i.e. metal vs. semicond.) but normally to be a negligible effect.

—

Combine Emission Cleavage Criterion on a single diagram:



Ductile/Brittle depends on loading mode as well as bonding type.

3-D

2D establishes Genl. mechanical stability.

But dislocations can be thermally activated out of crack tip, even when crack is stable against emission!

Activation barrier is set by critical loop of dislocation.

original estimate in Rice + Thomson.

Update: Thesis by Peter Anderson. Harvard Univ. (1986)

See also Argon, Acta Met, 35 185 (1987)

General

1. Dislocation self energy (includes image)
2. strain energy release.

From Hirth + Lothe.

$$U_{self} = \frac{1}{4}\mu b^2 r \frac{2-\nu}{8(1-\nu)} \ln \frac{8r}{e^2 r_0} \qquad \propto r$$

$$U_\sigma = -\frac{4}{3}\frac{\mu b^3}{\sqrt{1-\nu}} \sqrt{\frac{\gamma}{\mu b}}\, f(\theta, \hat{b}) \left(r^{3/2} - r_0^{3/2}\right) \propto r^{3/2}$$

$$U_{ledge} = \text{(Small term)}$$

Energy of act. is maximum in $U = U_{self} + U_\sigma + U_{ledge}$.

Original estimates on basis of whole b, and circular loop gave very large energies except for Fe. Experimentally, disl. are easier to produce.

ALSO there is a different slip system in general: (Non-Blunting)

Seen first by Burns + Webb, but ~~...~~ a genl. phenomenon - quantitative results by Michot on Si. Submitted to J. Matls. Res.

- cont. -

This whole question being revisited ...
See upcoming work, with Lin & Argon.

role of alternate slip plane.
role of high stress region on core size
role of partial b (w/o low energy stacking fault.)
role of non circular shape.

Can this problem be done properly (in at atomic level) in 3-D ??

TOUGHNESS & SHIELDING

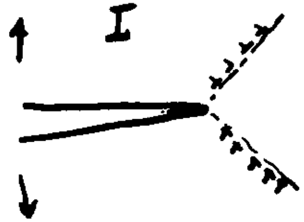
GEN'L IDEA

UNDERLYING CRACK: LOCAL & DETERMINES TOTAL O/A BEHAVIOR
for emission - k_e
for cleavage - k_c.

General Shielding Theorems

① "Natural" Dislocation Config.:

I



Dislocations for maximum Emission criteria

II

III

-cont-

Theorem on Shielding orthogonality (mixed mode).

Mode I dislocations only shield mode I loading –(no shielding of II + III.)

Exception –
In mode I, asymmetric dislocation emission induces (shields) mode II. (not mode III) (first noticed by Sinclair- Finnis – can be important effect for mixed mode problems. (i.e. serrated fracture found by Ohr)

A solvable many body Problem (B.C.S) (Dugdale)

Assume Mode III –

Assume force on dislocations is in balance:

$$f_d = \frac{Kb}{\sqrt{2\pi x}} - \frac{\mu b^2}{4\pi x} + \sum{}' \frac{\mu b b'}{2\pi} \frac{1}{x-x'} \sqrt{\frac{x'}{x}} = \sigma_f b$$

Assume continuum approx:

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

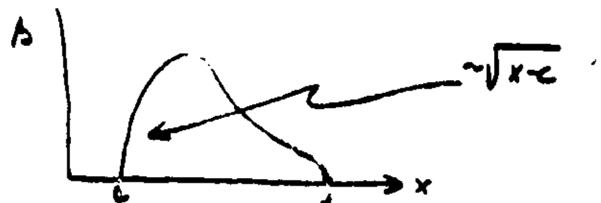
$$\sigma_f = \frac{K}{\sqrt{2\pi x}} - \frac{\mu \beta dx}{4\pi x} + \frac{\mu}{2\pi\sqrt{x}} \int_c^d \frac{\sqrt{x'}\,\beta(x')}{x-x'} dx'$$

$$\frac{2\pi}{\mu}\left[\sigma_f \sqrt{x} - \frac{K}{\sqrt{2\pi}}\right] = \int \frac{\sqrt{x'}}{x-x'} \beta(x')\, dx'$$

Hilbert Xform – see Muskhelishvili (details in SSP - Appendix)

$$\beta(x) = -\frac{2}{\mu\pi} \sqrt{\frac{(x-c)(d-x)}{x}} \int_c^d \frac{\left(\sqrt{x'}\,\sigma_f + K/\sqrt{2\pi}\right)\sqrt{x'}}{(x'-x)\sqrt{(x'-c)(d-x')}}\, dx'$$

This is an eliptic integral – Interested in asymptotic range c<<d:



For $c \ll d$

$$k = \frac{3}{\pi}\left(\frac{2}{\pi}\right)^{1/4} \sigma_f \sqrt{c}\left(\ln\frac{4d}{c}+\frac{4}{3}\right)$$

$$k = K - \mu \int \frac{B(x')}{\sqrt{2\pi x'}}\,dx' = \text{local } k.$$

$$\left.\begin{array}{l} K = 2\sigma_f\sqrt{2d/\pi} \\ K = \mu B\sqrt{\pi/2d} \end{array}\right\}$$

Not dependent on c — comes from original Bilby-Cottrell-Smith treatment.

Rice Paradox

Let $c \to 0$. Then

$$k = 0$$

Eliminate d from last 2 eqns:

$$\frac{K^2}{2\mu} = \sigma_f B$$

The force to move crack + Disl. is just the force to move the dislocations! When $c=0$, this is a rigorous result.

This is a paradox because all the energy goes into moving the dislocations, and <u>NONE</u> int creating the broken bonds at the crack tip. This result is because the dislocations cancel the local k at the crack tip. In order for there to be a finite energy absorbtion at the crack tip, $c>0$ is required. (originally proved by Rice in a different way - see Rice Sendai Conf. on Fract.)

But is this a subtle point, or a crucial one?

The previous eqns can be written

$k \sim \sigma_f \sqrt{c}$ ← Set by cleavage or emission condition at tip

$\frac{K^2}{2\mu} = \sigma_f B$ ← Shielding relation

Connection is thru σ_f

What is c or Disl. Free Zone?
(there is controversy on this point – (Birnbaum))

- Clearest in experiments by Ohr.
- Fundamentally:
  It connects the atomic bonding condition at crack tip with the shielding zone. (It must exist — otherwise $k \to 0$!) and provides the bridge between macroscopic and microscopic + atomic properties.
- Physically it arises:
  Finite distance between sources for Dislocations near the tip. (Frank-Read sources — (Gerberich))
  Distance required for a dislocation to move from a tip before another can be emitted.
- See recent work by ~~[illegible]~~ Li + coworkers for simulation of DFZ.

The problem is – what determines the B? Suppose the B are created at external sources due to σ exceeding the local yield stress. Then, we need a yield – dislocation density relation – (a constitutive relation – work hardening)

Suppose
$$B = B_0 \sigma_f^{n}$$

Then
$$K^2 = 2\mu B_0 \left(\frac{k}{\sqrt{c}}\right)^{n+1}$$
$$\left[k = \sqrt{4\mu\gamma} \right]$$

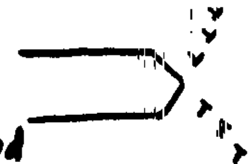
So the overall toughness of the material follows from:

1. strength of bonds (γ)
2. Dislocation response to stress.
3. Elastic constants.
4. Disl. Free zone

Touoness Perspective

Intrinsic Ductility/Brittleness

1. **Crack Emits**



Shape Change -
Dislocation dominated phenomenology. - Plastic failure

* Crack doesn't go any where !
Inherently high toughness + hi shielding

2. **Crack Cleaves**

* Crack is higly mobile - determined by local k. - i.e. state is unstable

Shielding can occur by natural dislocations - not too effective

Extrinsic Ductility

Crucial Issue:

Can a brittle crack induce such large amounts of external plasticity that over all ductile failure occurs

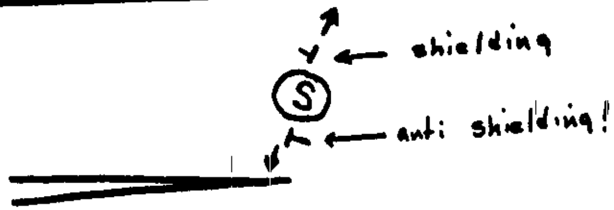
This means:

Local k never rises to k_c because there always exists a source nearby which produces shielding dis/.

? ? ?

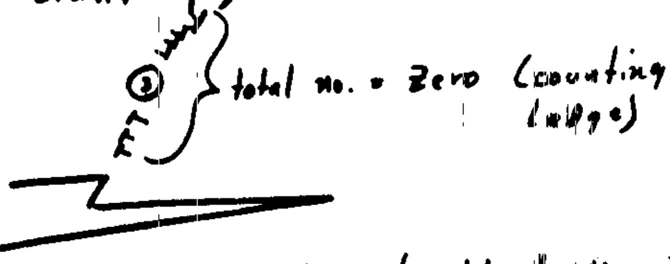
[This mechanism is proposed by Ashby + Embury as a serious mechanism for ductile Xtion (Scripta Met)]

<u>Some qualitative thoughts:</u>



1) <u>Thus</u>, <u>the</u> <u>initial</u> <u>action</u> <u>is</u> <u>anti shielding</u>
   This means that externally generated dislocations are always less effective in shielding than intrinsically produced dislocations!

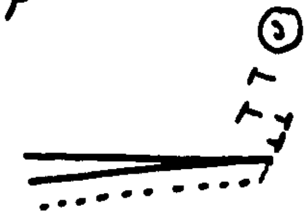
2) Then antishielding dislocations are absorbed, + net effect is shielding (and some non local blunting)

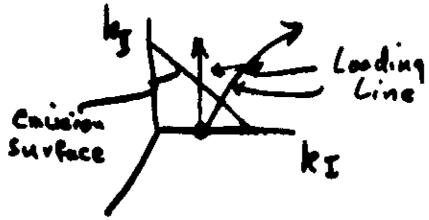


<u>Note</u>: probability to blunt tip is low!

3) Anti shielding dislocations change emission condition at tip

[k_{II} generated]





emission creates a dipole configuration near tip — ~~shifts~~ cancelling k_{II} and anti shielding. Then overall effect is shielding, + k_I goes negative, stabilizing cleavage crack

4) As k increases, crack again cleaves (even tho blunted!) and cycle is repeated

5) This process is <u>highly</u> rate sensitive!

<u>Conclusion</u> <u>The</u> <u>question</u> <u>is</u> <u>still</u> <u>open</u>

Mixed Cases

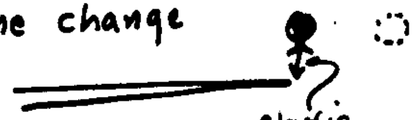
It now appears that a brittle crack has a low energy of activation for dislocation nucleation (?)

Thus as T increases, dislocation emission becomes significant, and ductility ensues. Si is such a case (Fe may be) – now being worked out.

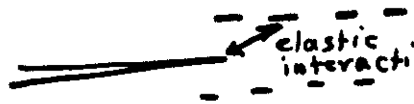
Mechanisms for Shielding Local Crack Tip in Ceramics

1. Dislocations
   Sources external → (some anti shielding)
   Source is crack → *much* more effective.

2. Transformation of Second Phase
   Stress induced volume change



3. Microcracking in polycrystals



* 4. Encapsulated Particle or Grain

(**) 5. Fiber "Reinforcement"

$K_c \to \infty$!

Concluding Summary

Emerging Possibility: Materials Design

THEORY

1) Enhanced modeling of crack structure because force laws now tractible.

2) Enhanced computation capability for more realistic crack-dislocation cloud simulation

3) Tailoring of materials thru enhanced processing controls (i.e. composites, quenched phases, etc.)