INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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SMR.550 - 35

SPRING COLLEGE IN MATERIALS SCIENCE ON
"NUCLEATION, GROWTH AND SEGREGATION IN MATERIALS SCIENCE AND ENGINEERING"
(6 May - 7 June 1991)

FRACTURE - I

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These are preliminary lecture notes, intended only for distribution to participants.

FRACTURE

- Observational Basis
  - (Ductile - Brittle Duality)
  - Hints for understanding
- Elasticity
  - General
  - Crack + Dislocation fields
  - Configurational forces
  - Shielding of Cracks.
- Atomic + Discrete Lattice Theories
  - Qm. force laws
  - Lattice structure of Defects
  - Greens Fns.
  - Cracks : Chemical effects at crack tip
- Ductility
  - Dislocation Emission (Intrinsic Brittlen
  - Extrinsic Ductility
    - Ductile Transitions
    - Shielding - Anti shielding
- Cracks at Interfaces
  - Elastic
  - Atomic / Discrete

Coworkers
I. H. Lin
V. Tewary
S. Zhou
K. Masuda - Jin
A. King
H. Zheng
W. Curtin

Mechanical Failure

Structural materials

Economic value / loss.

Bridge failures
Aircraft failures   Hi Tech
Gas + oil pipelines
Nuclear pressure vessels   Hi Tech
Space Appls.   Hi Tech
El. Devices   " "

High Tech:
Tradeoff of performance / Risk
Requires precise assessment.

Practice

1. Initial design requirements - Matl nominal prop.

2. Processing Quality Control
   Flow control (NDE)

3. In-use Monitoring (NDE)

NDE

Engineering Practice

1. Flaw Detection + charization
   Flaw size / shape (crack/void)
   critical size: 1 μm – ½ m.

2. Must know characteristics of flaw growth.
   Critical size/stress
   chemical environment
   Growth under cyclic Stress

FRACTURE MECHANICS

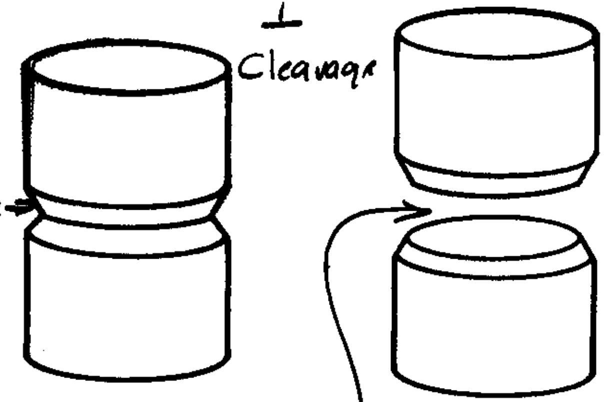
Specification of matls in terms of critical toughness tests

J-integral / COD / K_{Ic}

What Role for Fundamental Knowledge

NEW
What makes matls tough?
Role of external chem. Environ.
[illegible]

mica
SiO_2 glass
Si
Diamond
etc.

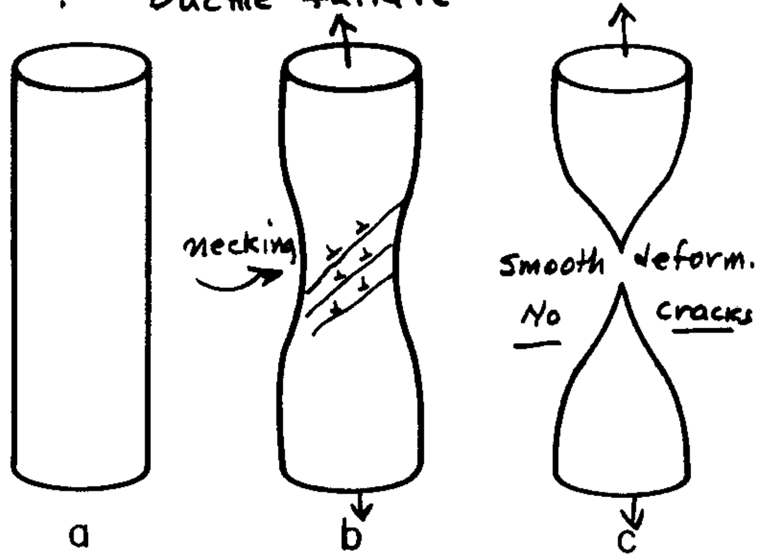


atomically Smooth cleavage
(No dislocations or other defect formation)

Failure Bipolarity

II
Ductile failure

"butter"
pure Cu, Al, etc.



Bipolarity

Brittle
High Strength

Ductil[e]
High
tough

Si, C, mica
etc.

pure Cu,
Al, etc.

technological materials balanced between high strength + toughness

Balance shifts with :

- strain rate
- Temperature
- chemical environment
- microstructure

Duality of Disl. + Cracks

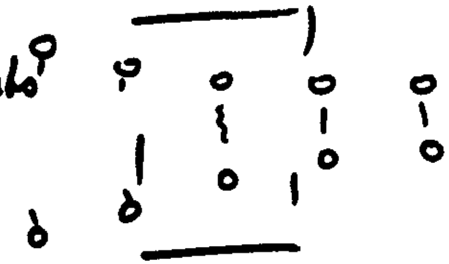
1. Why is $\sigma_y < \sigma_{th}$?

- Dislocation concentrates stress
- Dislaclation moves easily

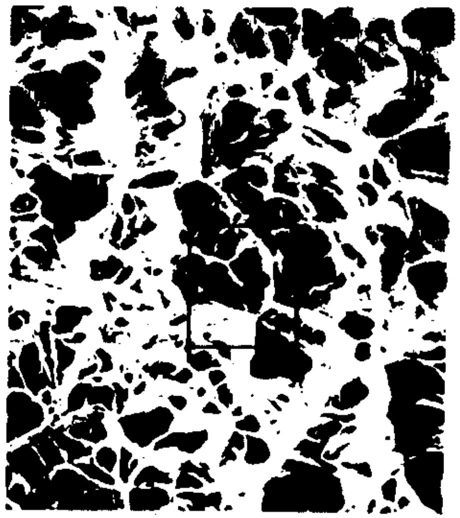
High Stress
$\approx \sigma_{th}$.

2. Why is $\sigma_c < \sigma_{th}$?

- Crack core concentrates stress
- Crack extends easily (when l large!)

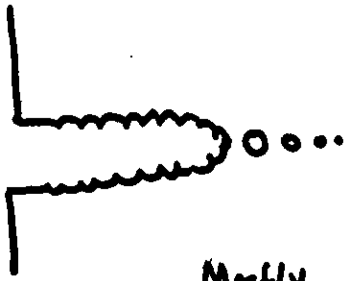


Hi Stress
$\approx \sigma_{th}$.



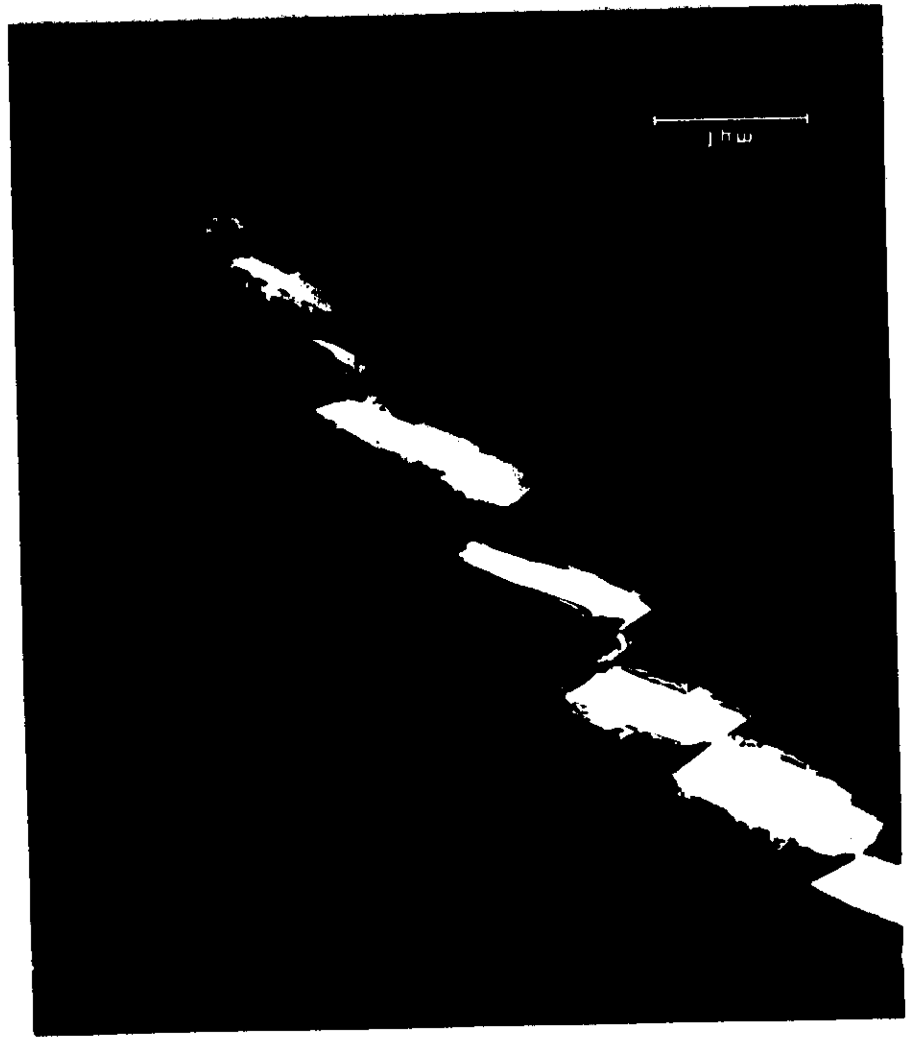
"Fracture" of a Techn. Matl. (Fe)

(8)



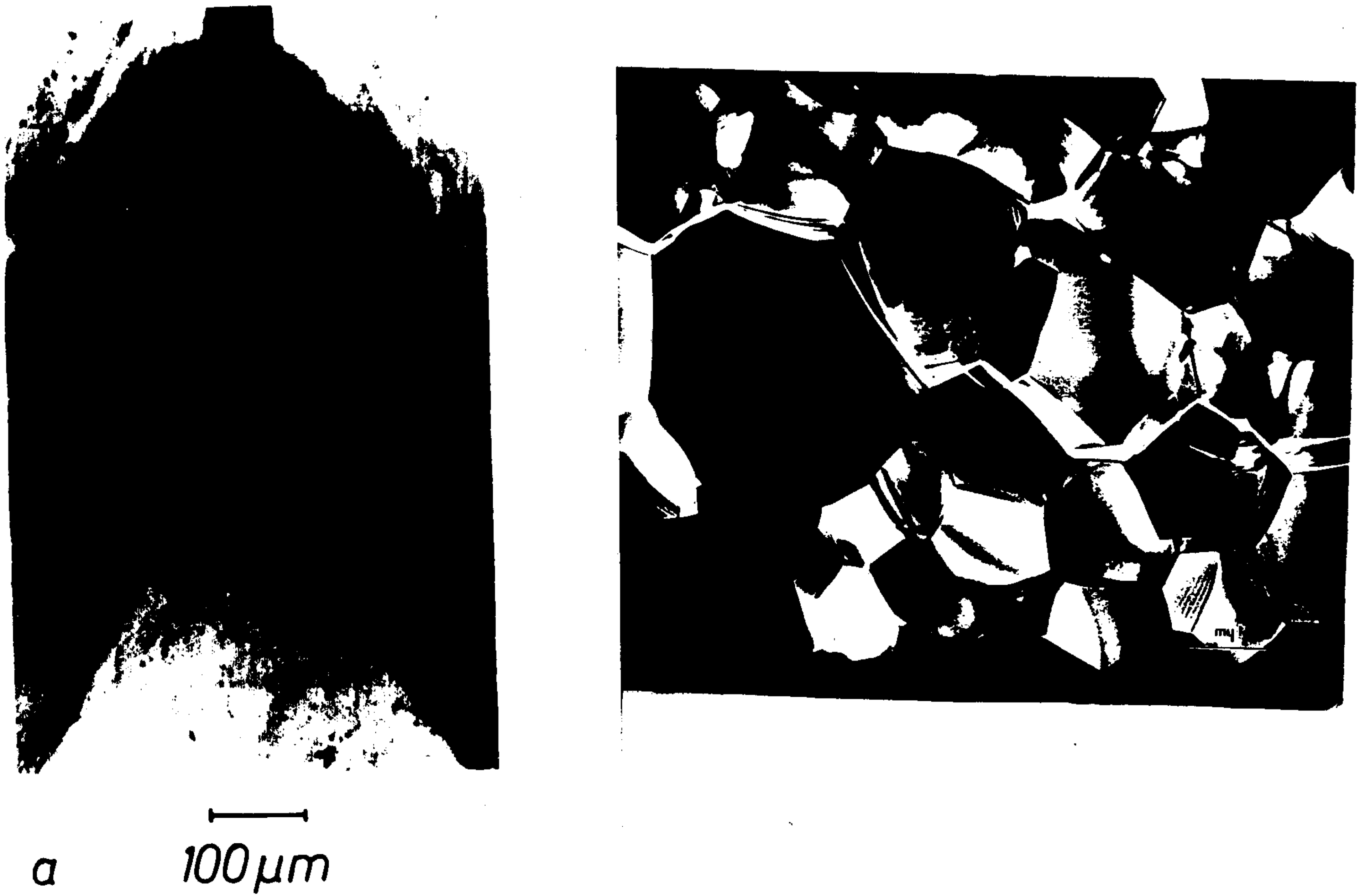
<u>Mostly</u> a ductile process.

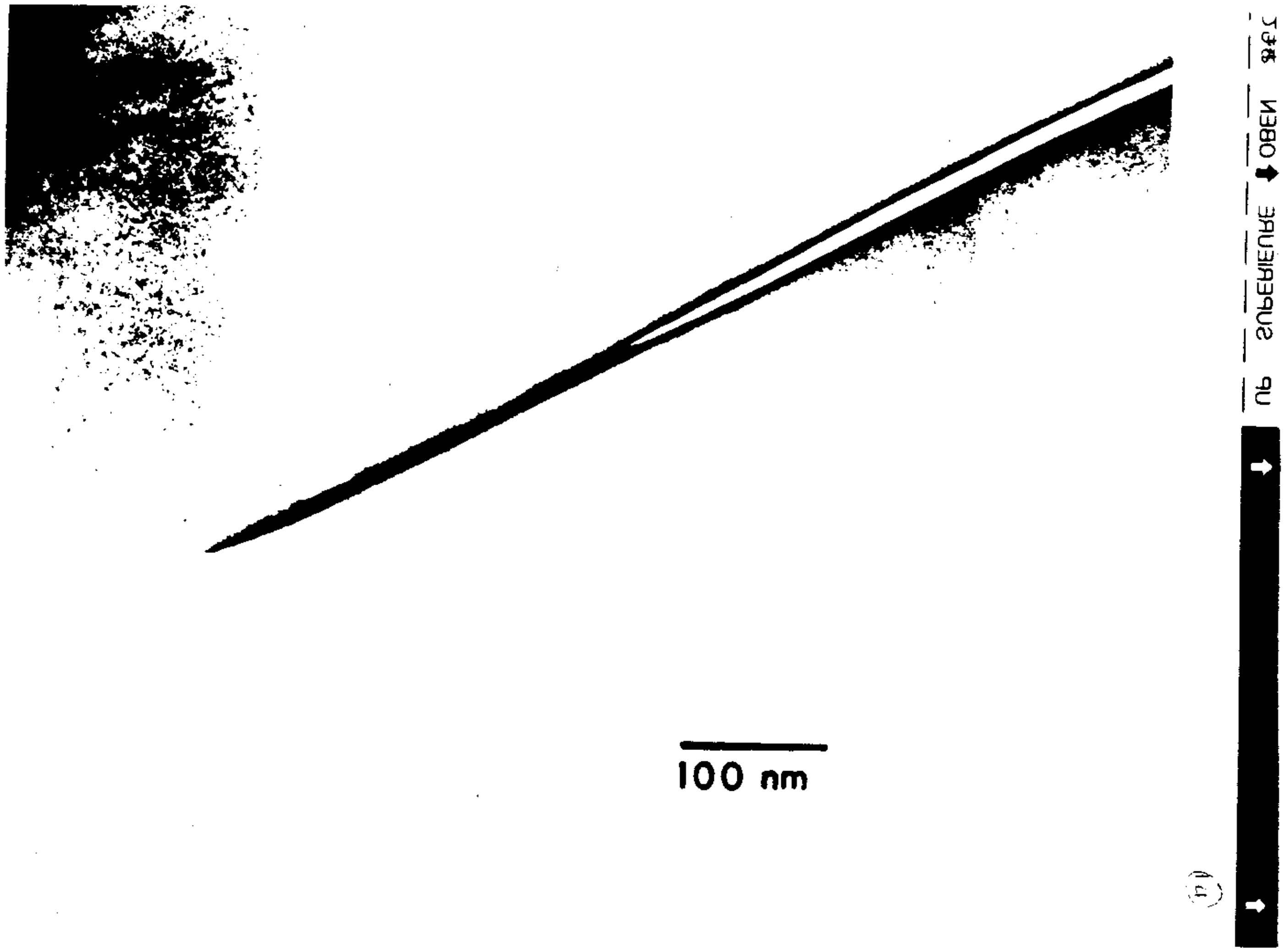
1. Initiation of holes / voids
2. Growth of voids by pure deformation shear processes. (shear bands, shear cracks ???)



b) 100µm

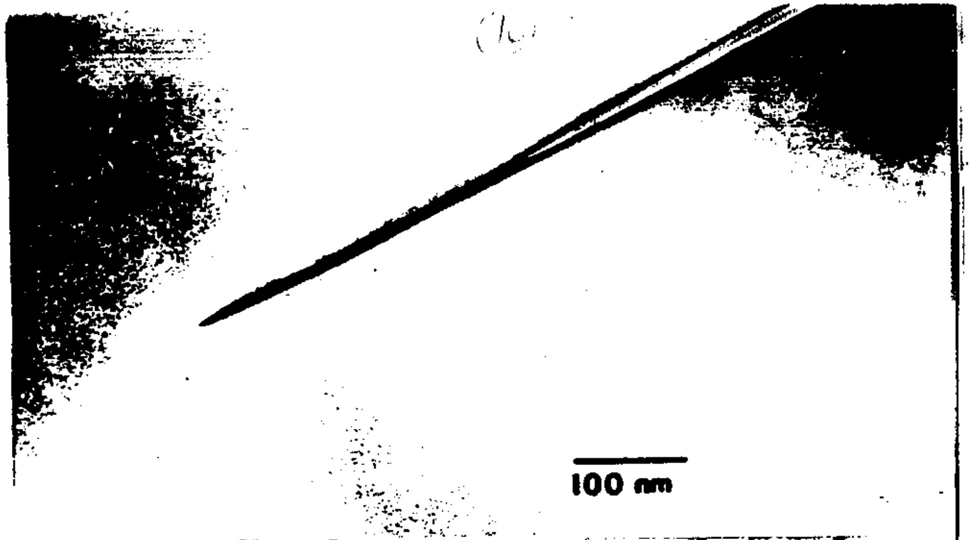
(12)

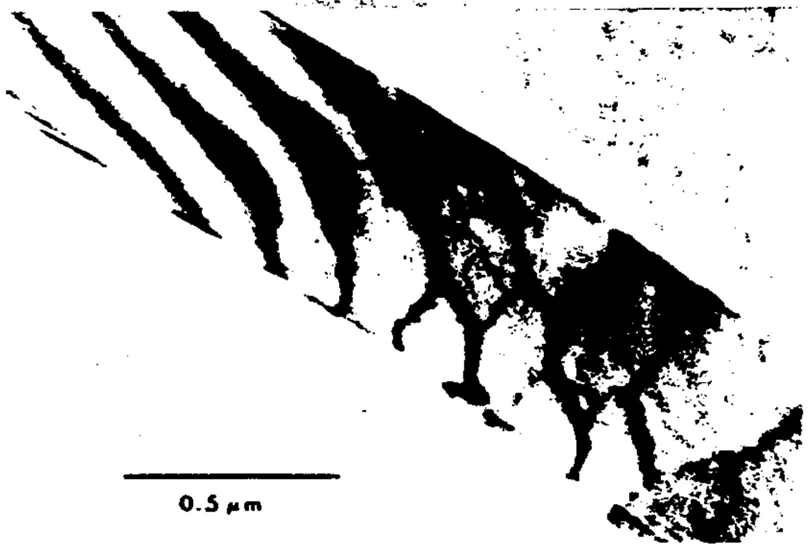


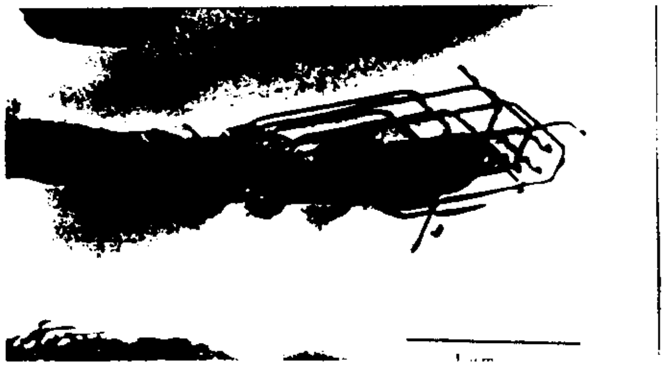

(a)
100 nm

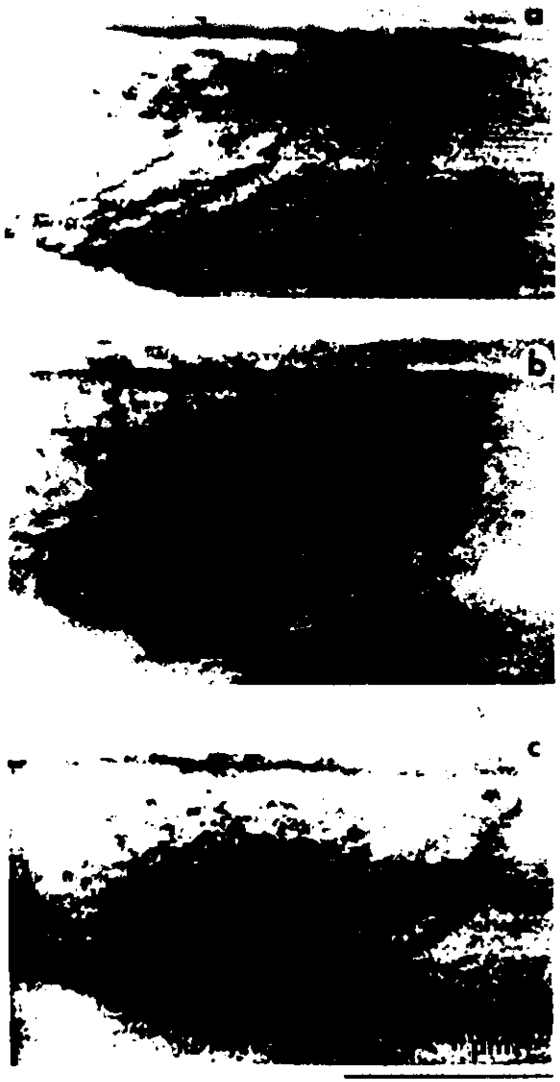

(b)
1 μm

Chia + Clarke (Acta Met) 17









(A)

(B)

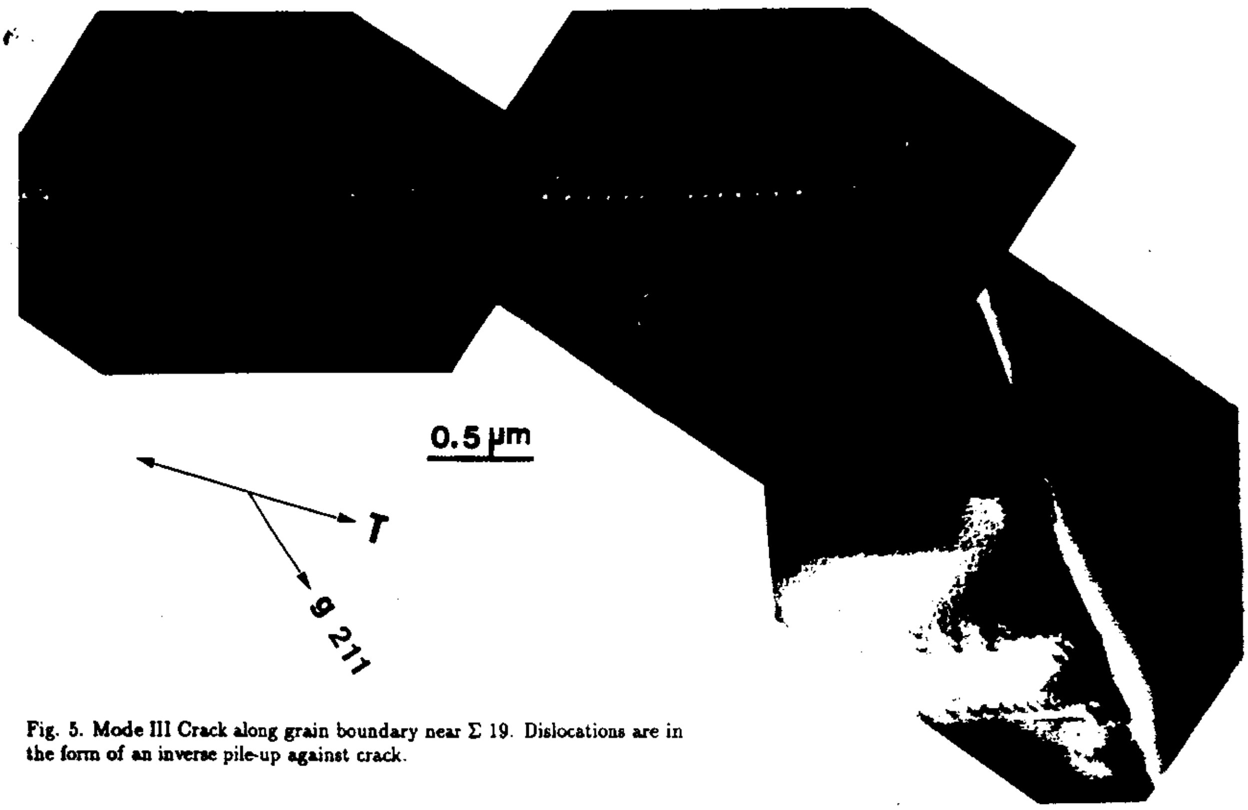
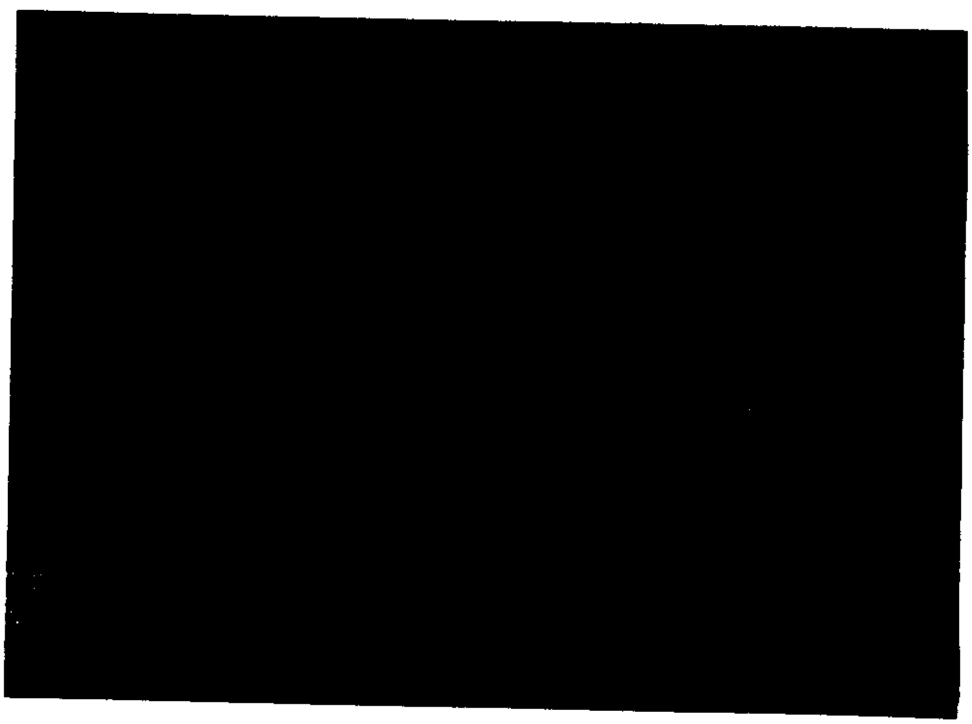
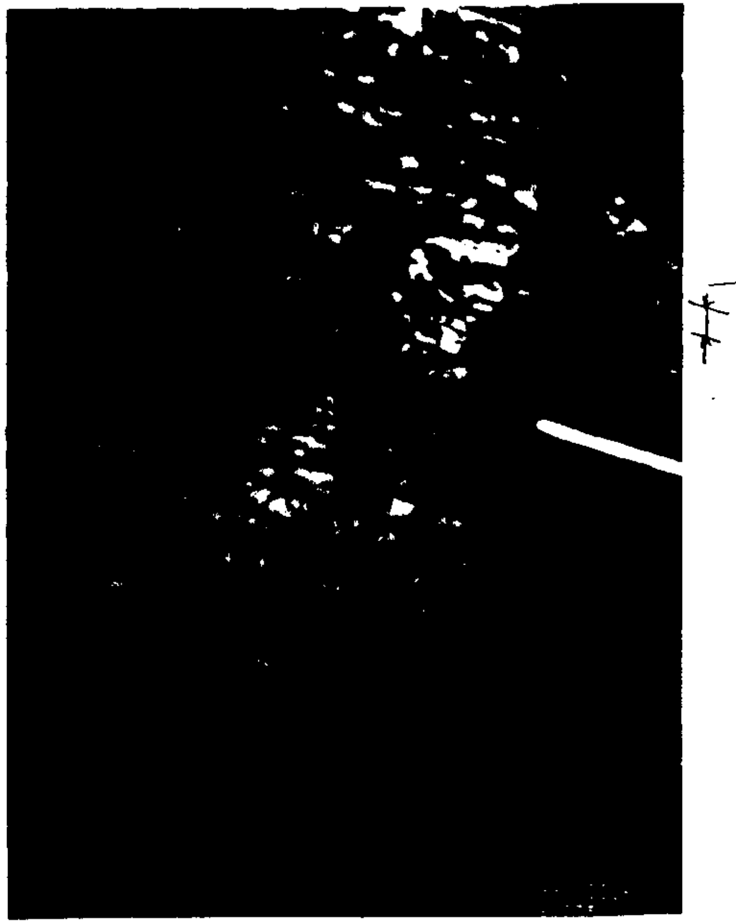


Fig. 5. Mode III Crack along grain boundary near Σ 19. Dislocations are in the form of an inverse pile-up against crack.



100 Å Cu / 100 Å Ni



100 Å Cu/ 100 Å Ni
potentiostatic

A Hint

Classification Scheme for Cracks

Atomic Crack

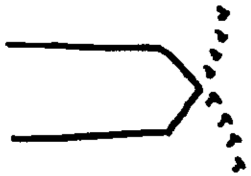
(Cleaving)

hi mobility
Lo resistance

$\sigma \propto \frac{k}{\sqrt{r}} \quad f = k^2$

Shielded by disl. $\quad k = K + K^D$

Emitting Crack



"zero" mobility
Zero force
moves only by emission

$\sigma \propto \frac{1}{r^p} \quad p > \frac{1}{2}$

Absorbing Crack

"zero" mobility
zero force
moves by Plastic opening

σ not singular
(but stress concentration)

<u>Again</u> No pure cases — understand how one relates to another.

Conclusions

- "Pure" cases exist, but as a rule, cracks AND dislocations coexist + interact
- Relative toughness depends on crack/dislocation interactions

  Direct dislocation/crack interact.

  Crack as source of Disl.
- External Chemicals modify crack/disl. intera

Tools

Elasticity (plasticity?) (ties to macroscopic)

Atomic scale theories / ideas

Bonding of defective Solids (force laws)

Microstructural characterization

el. Microscopy.

exper. study of crack structure Difficult

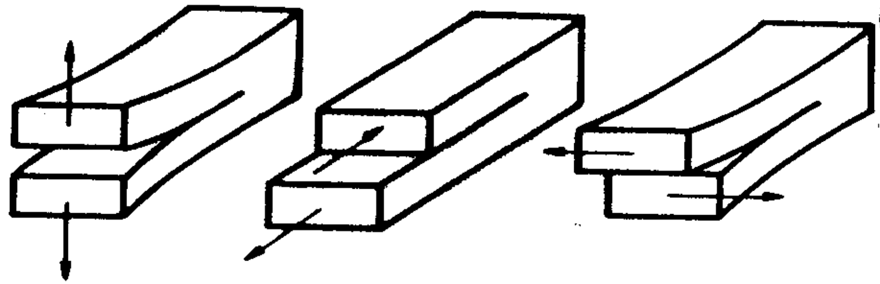
Disciplines

fract. Mech., Matls. Science, Physics

Chemistry

The Three Primordial Crack "Modes"

(Isotropic medium)



MODE I MODE II MODE III

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

Anti Plane strain (screw Xloc) (shear waves)

ELASTICITY

Gen. References

N. Muskhelishvili "Some Basic Problems in Mathetical Theory of Elasticity" Noordhoff Leiden (1977) (translation)

Timoshenko + Goodier "Theory of Elasticity" McGraw Hill (1970)

Specialized:

Kanninen + Popelar "Advanced Fracture Mechanics" Oxford. (1985)

de Velia, "Mekanica de Fractura" Monografia Techologica #1 Programa Regional de Desarrollo Cientifico y Tecnologico - OEA (198

Thomson, Solid State Physics Vol 39 (1986)

Anisotropic

Bacon, Barnett + Scattergood Progress in Matls. Sc. Vol 23 Pergamon, (1979)

Strain

Displacement : $\underline{u}(\underline{x})$ $\quad u_i(x_j)$

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \qquad \text{Strain}$$

$$\omega_{ij} = \frac{1}{2}(u_{i,j} - u_{j,i}) \qquad \text{Rotation}$$

First Order Theory

$$u_i(x_i + \delta x_i) = u_i(x_i) + (\epsilon_{ij} + \omega_{ij})\,\delta x_j + O(\delta x^2)$$

↑ Higher order elastic terms.

Engineering Strain

$$\gamma_{ij} = 2\epsilon_{ij} \quad i \neq j.$$

Stress

Stress is a force exerted across of surface inside or on body of a body.

Arises because of the stiffness of a body. (solid or liquid)

Assume the force is proportional to the surface area.

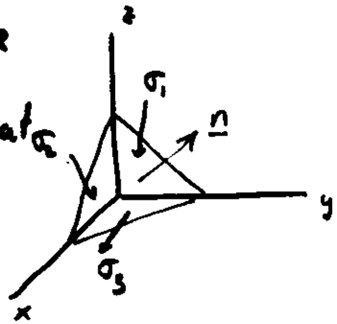
force = $F\,dS$

= "Traction"

Define

Traction: Force acting across a surface - Positive Exerts on Negative

Balance of Forces on a Volume



Define a function, $\sigma(x_i)$, such that the traction on OZY is σ_1, etc. i.e.

$T_{OZY} = \underline{\sigma_1}\, dA_{OZY} = \underline{\sigma_1 n_x}\, dS$

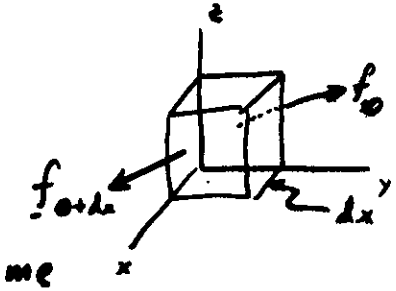
Add all tractions – must add to zero.

Thus, traction on XYZ is

$$\boxed{f_i = \sigma_{ij} n_j}$$

Def. of stress tensor fn. f_n is traction on dS

Equation of Equilibrium
(Elastic Field Eqn.)



$$\underline{f}_x(x+dx) = \underline{f}_0 + \frac{\partial f}{\partial x}\,dx$$

Thus total force on volume $dx\,dy\,dz$ is

$$\frac{\partial \sigma_{ix}}{\partial x} + \frac{\partial \sigma_{iy}}{\partial y} + \frac{\partial \sigma_{iz}}{\partial z} = \text{net stress force on } dV.$$

If a "body force" exists, (weight, electri forces, etc.) Then

$$\boxed{\sigma_{ij,j} = f_{body}}$$

Transformation of Coordinates

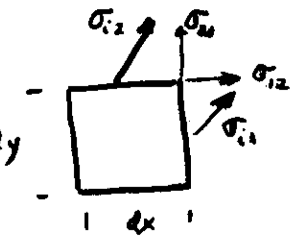
If Coordinates are transformed, (rot

$$dx_i' = S_{ij}\, dx_j$$
$$f_i' = S_{ij}\, f_j$$
$$\sigma_{ij}' = S_{ik} S_{jl}\, \sigma_{kl}$$
$$\epsilon_{ij}' = S_{ik} S_{jl}\, \sigma_{kl}$$

(Note: no con variant – covari distinction for rotations)

Symmetry of σ_{ij} ; Boundary Condition

If for an arbitrary volume, torque is zero, then



$$(\sigma_{21}\, dx)\, dy = (\sigma_{12}\, dy)\, dx$$

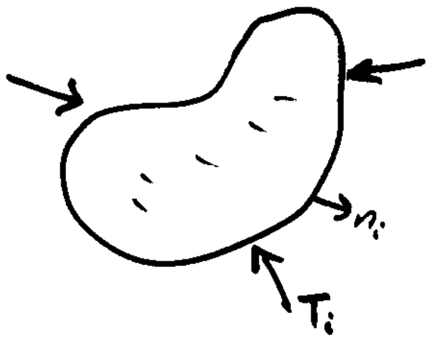
$$\sigma_{21} = \sigma_{12}$$

etc.

$$\boxed{\sigma_{ij} = \sigma_{ji}}$$

Boundary Condition on Stress.

If T_i is <u>External</u> force (traction) on body.



$$\boxed{\sigma_{ij}\cdot n_j = T_i}$$

Constitutive Relations : Hooke's Law

<u>Assume</u> a linear force/response Relation

$$\sigma_{ij} = C_{ijkl}\,\epsilon_{kl} \qquad (3^4 = 81 \text{ c's.})$$

But $\sigma_{ij} = \sigma_{ji}$; $\epsilon_{kl} = \epsilon_{lk}$

$$C_{ijkl} = C_{jikl} = C_{ijlk} \qquad (36 \text{ c's})$$

Also

$$C_{ijkl} = C_{klij} \qquad \text{(From energy)}$$

(21 c's in gen'l)

Energy Density Fn.

$$\frac{dE}{dt} = \oint \sigma_{ij}\,\dot u_i\, dS_j = \int (\sigma_{ij}\,\dot u_i)_{,j}\, dV$$

since $\sigma_{ij,j} \to 0$.

$$\frac{dE}{dt} = \int \sigma_{ij}\,\dot\epsilon_{ij}\, dV$$

Or per unit small volume

$$dE = \sigma_{ij}\, d\epsilon_{ij}$$

cont

or to integrate from zero strain to final Strain,

$$d\mathcal{E} = C_{ijkl}\, \epsilon_{ij} d\epsilon_{kl}$$

$$\boxed{\begin{aligned}\mathcal{E} &= \tfrac{1}{2} C_{ijkl}\, \epsilon_{ij}\, \epsilon_{kl} \\ &= \tfrac{1}{2} \sigma_{ij}\, \epsilon_{ij}\end{aligned}}$$

quadratic form in ϵ's or σ's

(Note $C_{ijkl} = C_{klij}$)

Note

$$\sigma_{ij} = 2 \frac{\partial \mathcal{E}}{\partial \epsilon_{ij}}$$

which could have been taken as definition of σ.

Incompatibility

There exist 6 ϵ_{ij}, but only 3 u_i. Hence the strain components overdetermine a solution. A single valued function, $u_i(x_j)$ exists if the rotation is single valued, i.e.

$$\oint \omega_{i,n}\, dl_n = 0.$$

But

$$\omega_i = \tfrac{1}{2} \epsilon_{ijk}\, u_{j,k}$$

$\epsilon_{ijk} \equiv$ completely anti symmetric tensor.

$\epsilon_{123} = -\epsilon_{213} = 1$, etc

And

$$\omega_{i,n} = \epsilon_{ikl}\, e_{ln,k}$$

$$\oint \epsilon_{ijl}\, e_{ln,k} = 0.$$

Or Curl [ ] = 0 ;

$$\boxed{-\epsilon_{ikl}\, \epsilon_{jmn}\, e_{ln,km} = 0} \quad \boxed{= I}$$

I = incompatibility − (Burgers vector).

Reduced Notation + Isotropic Elast.

$$C_{ijkl} \Rightarrow C_{ij}$$

$11 \to 1$
$22 \to 2$
$33 \to 3$
$23 \to 4$
$31 \to 5$
$12 \to 6$

$$(\gamma_{ij} = 2\epsilon_{ij} \quad i \neq j)$$

$$\sigma_{ij} = C_{ij} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \gamma_4 \\ \gamma_5 \\ \gamma_6 \end{pmatrix}$$ → Note!

Cubic

$$\begin{matrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{matrix}$$

3 constants

Isotropic

$$\begin{matrix} \lambda+2\mu & \lambda & \lambda & & & \\ \lambda & \lambda+2\mu & \lambda & & & \\ \lambda & \lambda & \lambda+2\mu & & & \\ & & & \mu & & \\ & & & & \mu & \\ & & & & & \mu \end{matrix}$$

2 Constants

$$\boxed{\sigma_{ij} = \lambda \delta_{ij} u_{l,l} + \mu (u_{i,j} + u_{j,i})}$$ Isotropic Elasticity

2D Elasticity $\left(\frac{\partial}{\partial z} = 0\right)$

Two Orthogonal Solutions

Anti Plane Strain (shear waves)

$u_3 \neq 0 \quad u_1 = u_2 = 0. \quad \left(\frac{\partial}{\partial z} = 0\right)$

$u_3(x_1, x_2)$ $\quad \sigma_{31,1} + \sigma_{32,2} = 0 \Rightarrow \mu(u_{3,11} + u_{3,22}) = 0 \Rightarrow \mu \nabla^2 u_3 = 0$

Introduce Complex Variable $x_1 + x_2 = z$

Equilibrium (Field Eqns)

$$\nabla^2 u = 0$$

Then $u = \frac{2}{\mu} \operatorname{Im} \eta(z)$

Hooke's Law becomes

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

$\eta(z)$ any complex fn. satisfying BC.

$$\sigma_{r3} = \operatorname{Im}(\sigma e^{i\theta})$$

$$\sigma_{\theta 3} = \operatorname{Re}(\sigma e^{i\theta})$$

Singular Solutions (2D)

Crack Problem

Desire a function such that

$$\text{Real}\{\eta'(z) = 0\} \quad x_1 < 0.$$

$\underline{\underline{\sigma}} \cdot \underline{n} = 0$;

$\sigma_{32} = 0 \quad x_1 < 0.$

$$\eta' = z^{n/2} \qquad n = \pm 1, 3, \cdots$$

Requirements

Energy enclosed at origin finite

$$\int \sigma^2 dA = \int \sigma^2 r\, d\theta \ ; \ (r\sigma^2) \to 0 \text{ at } \Sigma_0.$$

$\sigma \to 0$ at ∞

Thus

$$\boxed{\sigma = \frac{K}{\sqrt{2\pi z}}}$$

CRACK $\quad \eta' = \dfrac{K}{2\sqrt{2\pi z}}$

K is Stress Intensity Factor

Displacement on $x_1 < 0$

$$u_3 = \frac{2}{\mu} \operatorname{Im} \eta = \operatorname{Im} \sqrt{\frac{z}{\pi}}\, K \sqrt{z}$$

On $x_1 < 0 \quad u_3 = \pm \sqrt{\dfrac{2x}{\pi}}\, K$

Dislocation

$$\int u\, dl = b$$

(Incompatiblity source)

⊥

Log functions have desired property.

$$\log z = \log|z| + i\theta$$

$$\boxed{\eta(z) = \frac{\mu b}{4\pi} \ln z}$$

$$\boxed{\sigma(z) = \frac{\mu b}{2\pi z}}$$

Dislocation

Point Force

1. External Force F
2. Surrounding material exerts force

   $$\int \sigma_{r3}\, r\, d\theta$$

   on material enclosed. (note sign of $\underline{n}$)
3. Total force on enclosed matter $= 0$.

   $$-\int \sigma_{r3}\, r\, d\theta = F$$

If $\boxed{\sigma = -iF/2\pi z} = -iFe^{-i\theta}/2\pi r$; $\sigma_{r3} = \dfrac{-F}{2\pi r}$

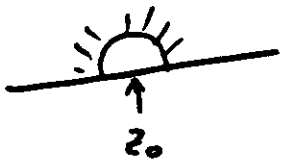
Then Integration is satisfied.

$\boxed{F = F_z}$

Green's Function for Crack

A crack stress field must be generated by an extern stress field. Otherwise nothing opens the crack. These forces may be applied to open surfaces of the crack, or to actual external surfaces of the specimen. (In the latter case, the solution will depend on shape of specimen.)

For an ∞ surface



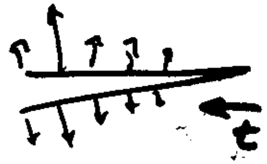
This is ½ previous problem of Point force.

$$\eta'_{\binom{\text{half}}{\text{plane}}} = \frac{F}{2\pi(z-z_0)i}$$

To satisfy BC for crack, must have $1/\sqrt{z}$ at crack tip. Thus, multiply by $\sqrt{z_0/z}$. Then near z_0, have point force, near crack, get necessary $1/\sqrt{z}$

$$\boxed{\eta' = \frac{\ }{2\pi(z-z_0)i}\sqrt{\frac{z_0}{z}} \quad \text{UNIT FORCE.}}$$

General Solution for loaded semi ∞ crack



$$\sigma(z) = \frac{1}{\pi\sqrt{z}}\int_0^\infty \frac{p(t)\sqrt{t}}{z+t}\,dt$$

singular for $(z) = -t$

$p(t)$ is stress distribution on crack surface. (σ_{22})

NOTE $P(t)$ is equal + opposite on the two surfaces.

(forces which are in same sense on the two surfaces correspond to surface stress — not discussed)

Because of crack loading, a K-field is generated

$$K = \lim_{z\to 0}\sqrt{2\pi z}\,\sigma(z) = \sqrt{\frac{2}{\pi}}\int_0^\infty \frac{p(t)}{\sqrt{t}}\,dt$$

Dislocation + Crack

Method of Solution

1. Note crack surfaces must be traction free. i.e. $\sigma_{32} = 0 \quad x_1 < 0$.
2. But Dislocation in free space generates a stress on $x_1 < 0$.
3. Add stresses which cancel the stresses on $x_1 < 0$.

$$\sigma = \sigma_0 + \sigma_1$$

$$\sigma_0 = \frac{K}{\sqrt{2\pi z}} + \frac{\mu b}{2\pi(z-\xi)}$$

$$\sigma_1(z) = \frac{1}{\pi\sqrt{z}} \int_0^\infty \frac{[-Re\{\sigma_\perp\}]_{crack}\sqrt{t}}{z+t}\,dt$$

$$-Re\{\sigma_\perp\} = \frac{\mu b}{2\pi} \frac{t + \frac{\xi+\bar{\xi}}{2}}{(t+\xi)(t+\bar{\xi})}$$

Final

$$\sigma = \frac{K}{\sqrt{2\pi z}} + \frac{\mu}{4\pi\sqrt{z}}\left(\frac{b}{\sqrt{z}-\sqrt{\xi}} - \frac{b}{\sqrt{z}-\sqrt{\bar{\xi}}}\right.$$

$$= \frac{K}{\sqrt{2\pi z}} + \frac{\mu b}{4\pi}\cdot\left[\frac{1}{z-\xi}\left[\sqrt{\frac{\xi}{z}}+1\right] + \frac{1}{z-\bar{\xi}}\left[\sqrt{\frac{\bar{\xi}}{z}}-1\right]\right]$$

PLANE STRAIN

Mathematics is generally similar — But more complicated.

Use complex variable. Need a function which represents stress as before. But there are 3 independent stress $\sigma_{11}, \sigma_{22}, \sigma_{23}$. Hence need $\underline{\underline{2}}$ fns.

Plane Strain

$u_3 \equiv 0. \qquad u_1, u_2.$

$\sigma_{3i} \equiv 0. \qquad \sigma_{11}, \sigma_{22}, \sigma_{12}$

The two complex functions describing ple strain are from Goursat.

1. Write Equil. Eqns: $\nabla\cdot\sigma = 0$.

$$\sigma_{11,1} + \sigma_{12,2} = 0$$

$$\sigma_{22,2} + \sigma_{12,1} = 0.$$

These are same as:

$$\frac{\partial}{\partial z}\left[\sigma_{11} - \sigma_{22} + 2i\sigma_{12}\right] + \frac{\partial}{\partial \bar{z}}\left[\sigma_{11} + \sigma_{22}\right] = 0$$

The form of solution shows an extra "$\frac{1}{\sqrt{z}}$" contribution from Dislocation.

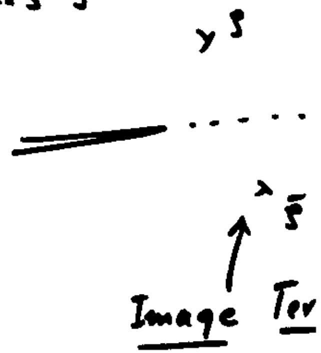
This is termed SHIELDING of crack by Dislocation —

<u>Thus</u>

$$K = k + k^D$$

K: "out side"; k: local crack; k^D: Dislocation term

$$k^D = \frac{\mu b}{2}\left[\frac{1}{\sqrt{2\pi\xi}} + \frac{1}{\sqrt{2\pi\bar{\xi}}}\right]$$



Shielding Depends on Sign of b.

Shielding	$b > 0$
Anti shielding	$b < 0$

(see Prof Lung)

The two terms are independent.

Second is real. + in terms of a $\phi(z)$,

$$\sigma_{11} + \sigma_{22} = 2\left(\varphi'(z) + \overline{\varphi'(z)}\right)$$

By integration of first [ ]. See (Appendix A)

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

$\varphi + \psi$ are now two independent complex fns. from which stresses (and displacements) can be obtained. Use a different pair, convenient for crack problem.

$$\left[\begin{aligned} \sigma_{11} + \sigma_{22} &= 2\left(\varphi'(z) + \overline{\varphi'(z)}\right) \\ \sigma_{22} - i\sigma_{12} &= \varphi' + \overline{\omega'} + (z-\bar{z})\,\overline{\varphi''} \\ 2\mu(u_1 + iu_2) = 2\mu u &= \kappa\varphi - (z-\bar{z})\,\overline{\varphi'} - \overline{\omega} \end{aligned}\right]$$

$\varphi + \omega$ are elastic potentials + are analytic compl fns.

—

Solution of Plane Strain Crack Problem.

$$(\sigma_{22}+i\sigma_{12})^+(-n^+) + F^+ = 0$$

$$(\sigma_{22}-i\sigma_{12})^+ = [\varphi'+\bar\omega']^+ = -\bar F^+$$

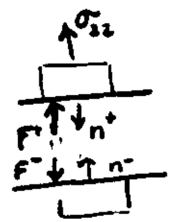
Likewise, on bottom

$$(\sigma_{22}-i\sigma_{12})^- = [\varphi'+\bar\omega']^- = \mp\bar F^-$$

Note, $F = F_{I} + iF_{II}$

mode I   mode II

$\sigma_{12}, \sigma_{22} = 0$ on neg. axis.



Load analysis - F is a Force distribution on the two cleavage surfaces.

$\varphi+\bar\omega$ is not an analytic fn. of z because of $\bar\omega$.

Define

$f(z)$ analytic

Then $f^*(z) = \overline{f(\bar z)}$

If $f = az + bz^2$,

$f^* = \bar a z + \bar b z^2 = f^*(z)$

Now on x_1 axis,

$$\overline{\omega(z)}\Big]_{x\,\text{axis}} = \omega^*(z)\Big]_{x\,\text{axis}}$$

Thus bc on crack:

$$[\varphi'(z)]^+ + [\omega'^*(z)]^- = -\bar F^+$$

$$[\varphi'(z)]^- + [\omega'^*(z)]^+ = \mp\bar F^-$$

Hence $\varphi'(z) + \omega'^*(z)$ has discontinuity on crack plane

$$[\varphi'+\omega'^*]^+ + [\varphi'(z)+\omega'^*(z)]^- = -2\bar F \qquad (F^+ = -F$$

But $\varphi'(z) - \omega'^*(z)$ is analytic every whe

$$[\varphi'(z) - \omega'^*(z)]^+_- = 0. \Rightarrow \varphi'(z) = \omega'^*(z)$$

Thus we require a function $\varphi+\omega$ which satisfy these b.c.

This is a Hilbert problem:

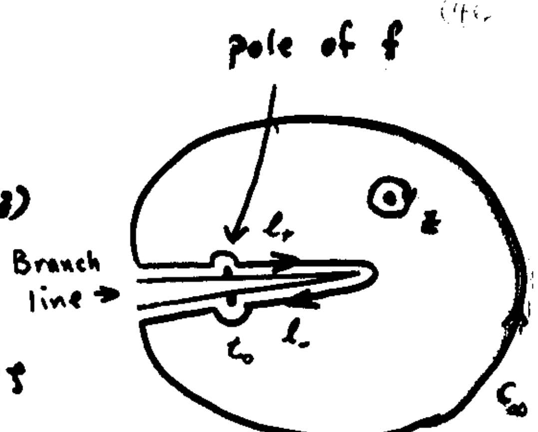
$$-\bar F = [\varphi(z)]^+ + [\varphi(z)]^-$$

$\varphi(z)$

$$\frac{[\varphi(z)]^+}{[\varphi(z)]^-}$$

Hilbert Problem

Cauchy Integral for $f(z)$



$$f(z) = \frac{1}{2\pi i} \int \frac{f(\zeta)}{\zeta - z}\, d\zeta$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{0} \frac{f(t)}{t-z}\, dt + \frac{1}{2\pi i} \int_{0}^{-\infty} \frac{f(t)}{t-z}\, dt$$

$$+ \frac{1}{2\pi i} \int_{C_\infty} \frac{f(\zeta)}{\zeta - z}\, d\zeta$$

If f is regular at ∞ the $\int_{C_\infty} = 0.$

$$f(z) = \frac{1}{2\pi i} \int_{-\infty}^{0} \frac{g(t)}{t-z}\, dt$$

$$g(t) = f^+ - f^- \quad \left\{ \begin{array}{l} g \text{ is discontinuity} \\ \text{at branch line.} \end{array} \right.$$

$\boxed{\text{If } g(t) \text{ is known on branch then } f(z) \text{ is known every where}}$

For crack, we have a discontinuity of form

$$\varphi'(z) + \omega'^*(z) = \chi(z)$$

where $\chi^+(z) + \chi^-(z) = h(t)$ on branch.

Musschelishvili Approach:

Find an "integration factor" which makes $h(t)$ have property of $g(t)$ ~~on branch~~

Thus

If $\quad [\chi(z)]^+ + [\chi(z)]^- = h(t) \quad$ (known)

Find $\Xi(z)$

$$\left[\frac{\chi(z)}{\Xi(z)}\right]^+ - \left[\frac{\chi(z)}{\Xi(z)}\right]^- = g(t) \quad \text{(known)}$$

It is not surprising to find $\sqrt{z}$ is an interesting function:

$$\frac{[\sqrt{z}]^+}{[\sqrt{z}]^-} = -1$$

We can therefore write

$$\sqrt{z}\left(\varphi' + \omega'^*\right) = \frac{1}{2\pi i} \int_{-\infty}^{0} \frac{2\,\overline{F}(t)\sqrt{t}}{(t-z)}\, dt$$

and we have derived a Green's function for the stress distribution on the cleavage plane.

Since

$$[\varphi'(z) - \omega^{*\prime}(z)]_-^+ = 0$$

$\varphi' - \omega^{*\prime}$ have no discontinuities. Hence

$$\varphi'(z) = \omega^{*\prime}(z) \quad \text{everywhere}$$

Thus

$$\left[\begin{aligned} \varphi'(z) = \omega^{*\prime}(z) &= \int_{-\infty}^{0} \bar{F}(t)\, g(z,t)\, dt \\ \eta'(z) &= \int_{-\infty}^{0} F_{III}\, g(z,t)\, dt \\ g(z,t) &= \frac{1}{2\pi i\,(t-z)}\sqrt{\frac{t}{z}} \end{aligned}\right]$$

Unified result for Mode III & Mode I, II. Thus, η' & φ' are on same footing as potentials for elastic 2D problem.

Now any problem in plane strain is solved in similar way as mode III, because Green's fn. are same. B.C. are always that $\varphi'(z)^+ + \varphi'^- = 2\bar{F}$

Crack K-fields

From the Green's Fns. the stress fld of the crack can be determined (For Green's Fns for a finite crac see SSP, p29)

From the Definition of K:

$$\bar{K} = \lim_{z \to 0} 2\sqrt{2\pi z}\;\varphi'(z)$$

$$K = K_I + i K_{II}$$

For a point force at t: $(t>0)$

$$\bar{K} = \sqrt{\frac{2}{\pi}}\,\frac{\bar{F}}{\sqrt{t}} \qquad F = F_I + i F_{II}$$

For finite crack – see SSP.

$$K = F\sqrt{\pi a} \qquad a = \tfrac{1}{2}\text{ crack } l$$

F = constant force

Dislocation Stress Fields

Definition of Dislocation

Thus φ and ω are double valued function with $\underline{b}$ discontinuity at origin

$$\oint \frac{du}{ds}\, ds = \underline{b}$$

Try

$$\varphi' = \frac{A}{z} \qquad \varphi = A \ln z$$

$$\omega' = \frac{B}{z} \qquad \omega = B \ln z$$

From Eqn for $u(z)$,

$$2\mu u = \kappa A \ln z - (z - \bar z)\,\frac{\bar A}{\bar z} - \bar B \ln \bar z$$

$$\Delta u = b = b_1 + i b_2 = \frac{\kappa}{2\mu}\, 2\pi i\, A + \frac{\bar B}{2\mu}\, 2\pi i$$

$$A = \bar B = \frac{\mu b}{\pi i (\kappa + 1)} \qquad \kappa = 3 - 4\nu.$$

Satisfies B.C. at origin – also gives $\sigma \to 0$ at ∞

But such a solution gives very strange translation properties. That is,

If $\varphi' = \dfrac{A}{z - \zeta}$,

$$\sigma_{11} - i\sigma_{12} = \frac{A}{z - \zeta} + \frac{A}{\bar z - \bar\zeta} - \frac{2 y \bar A}{(\bar z - \bar\zeta)^2}$$

not invaria

Hence, Add a term which makes third term invariant with traslation.

$$\varphi' = \frac{A}{z - \zeta} \qquad \omega' = \frac{\bar A}{z - \zeta} - \frac{(\zeta - \bar\zeta)}{(z - \zeta)^2} A$$

From these solutions for dislocation, can solve crack-dislocation problem.

$$\varphi' = \varphi'_{crack} + \varphi'_{xloc} + \varphi'_1 \ ; \ \omega' = \cdots$$

where φ'_1 chosen to make

$$\varphi' \to 0 \text{ on neg. real axis}$$

$$\left[\varphi'_1 = -\varphi'_{xloc}\right]_{\text{neg. axis}}.$$

See SSP. p 34. for details

Result is again the induced K-field at crack tip.

$$K^D = K_I^D + i K_{II}^D = \frac{i\mu}{2(1-\nu)} \left[\frac{b}{\sqrt{2\pi\xi}} + \text{[illegible]} + \frac{\pi \bar{b} (\xi - \bar{\xi})}{(2\pi \bar{\xi})^{3/2}} \right]$$

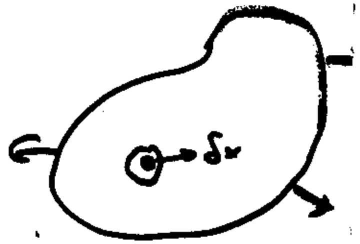
image term

"extra" complexity

Eshelby's Theorem: Force on Elastic Singul

SSP

3 stages to analysis



① Assume an energy density fn. exists [Single valued]

Assume the soln. is rigidly displaced.

$$W(x) = W_0 - \frac{\partial W}{\partial x_i} \delta x_i \qquad \delta x = \text{const. displ.}$$

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

② Resatisfy BC. on surface $(\sigma_{ij} \, dS_j = 0)$

Assume new stresses are added to surface. Satisfy the new BC. These generate additional displ., Δu_i

$$\Delta u_i = u_i^{\text{final}} - \underbrace{\left(u_i^0 - \frac{\partial u_i^0}{\partial x_j} \delta x_j \right)}_{\text{rigid disp part.}}$$

Work done by these stresses is

$$\delta U^2 = \oint (\sigma_{ij}^0 + \Delta\sigma_{ij}) \, \Delta u_i \, dS_j$$

$$\simeq \oint \sigma_{ij}^0 \, \Delta u_i \, dS_j$$

3) Final contribution is due to change in external sources of force on body of body (i.e. a weight might fall)

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

$$\delta U = \delta U^1 + \delta U^2 + \delta U^3$$

$$= - \int \left(W \delta_{ik} - \sigma_{ij} u_{j,k}\right) dS_k \, \delta x_i$$

$$\boxed{f_i = \oint \left(W \delta_{ik} - \sigma_{ij} u_{j,k}\right) dS_k}$$

Note

1. W need not be linear – But must be single valued fn. — other wise Gauss theorem invalid.
2. This is a 3-D result.
3. Independent of surface.

Proof of Surface independence:

$$f^1 - f^2 = \oint_{S_1 S_2} \left(W \delta_{kj} - \sigma_{ij} u_{i,k}\right) dS_j$$

$$= \int_{\text{enclosed Vol}} \left(W_{,k} - \sigma_{ij} u_{i,kj}\right) \qquad \sigma_{ij,j} = 0.$$

Now $W = \int \sigma_{ij}\, d\epsilon_{ij}$ If $\sigma_{ij}(\epsilon_{ij})$ – No explicit dep. on x.

$$W_{,k} = \epsilon_{lm,k} \frac{d}{d\epsilon_{lm}} \left[\int \sigma_{ij}\, d\epsilon_{ij}\right] = \epsilon_{lm,k}\, \sigma_{lm}$$

$$\epsilon_{lm,k} = \frac{1}{2}\left[u_{l,mk} + u_{m,lk}\right]$$

$$W_{,k} = \sigma_{ij} u_{j,ki}$$

QED.

Note 1) Independence depends on not having singularities between $S_1 + S_2$.
Again – elastic need not be linear. But matl must be homogeneous.
2) These theorems apply to cracks because integrand is either symmetric or zero

Force in 2D

Independence of f on contour is very reminiscent of Cauchy theorem.

Suggests the force is a property only of the singularity itself.

Thus

Convert the Contour integral by Cauchy theorem to a statement about residues of stress functions:

Plane Strain

$$\bar{f} = f_1 - i f_2 = \sum_{Res} \frac{2\pi(1-\nu)}{\mu}\Big[2\,Res\,(\varphi'\omega' - \varphi'^2 - z\varphi'\omega \ldots) + Res\,(\varphi^2)\Big]$$

Anti Plane Strain

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

These expressions are useful when dislocations + cracks interact.

Anti plane strain – especially simple. Plane strain. φ, ω, already given.

Simple cases

Dislocation:

$$\sigma = \sigma_0(z) + \frac{\mu b}{2\pi z} \qquad \text{(anti plane)}$$

$$\bar{f} = b\sigma_0 \qquad \text{(Peach-Koehler)}$$

(no self force!)!

Crack

$$\sigma = \frac{K_{III}}{2(2\pi z)^{1/2}} \qquad \text{(pure self f)}$$

$$\bar{f} = \frac{k_{III}^2}{2\mu} \qquad \text{(anti plane)}$$

Known as "Energy release rate" – Derived by Irwin

$$\bar{f} = \frac{1-\nu}{2\mu}\left(k\bar{k} + \frac{k^2 - \bar{k}^2}{2}\right)$$

$$f_1 = \frac{1-\nu^2}{E}\left(k_I^2 + k_{II}^2\right) = \frac{1-\nu}{2\mu}(\cdots$$

Climb force unphysical

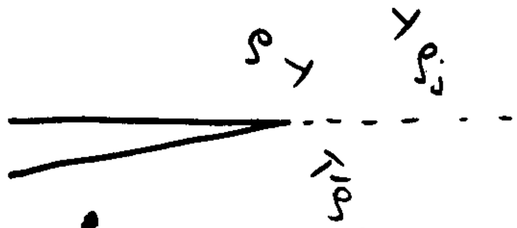
Dislocation force w/ crack.

(Mode III)

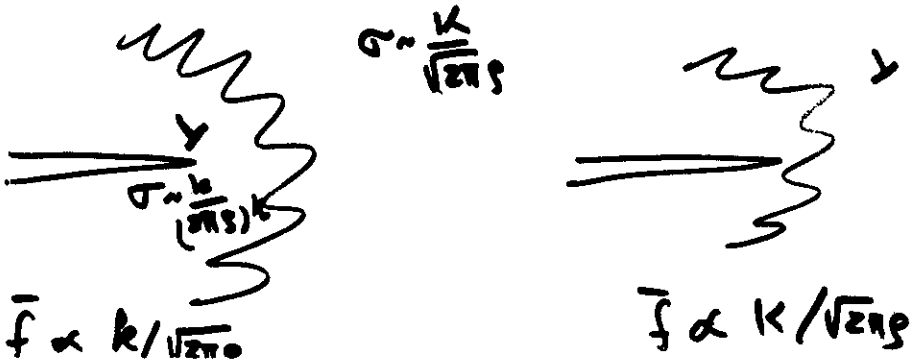
$$f = \underbrace{\frac{K_{III}\, b}{\sqrt{2\pi\rho}}}_{\text{[crack]}} - \frac{\mu b^2}{4\pi}\underbrace{\left[\frac{1}{2\rho} + \frac{1}{\rho-\bar\rho} - \left(\frac{\bar\rho}{\rho}\right)^{1/2}\frac{1}{\rho-\bar\rho}\right]}_{\text{[Image]}}$$

$$+ \sum_i \frac{\mu b b_i}{4\pi}\left[\frac{1}{\rho-\rho_j} - \frac{1}{\rho-\bar\rho_j} + \sqrt{\frac{\rho_j}{\rho}}\,\frac{1}{\rho-\bar\rho_j} + \sqrt{\frac{\bar\rho}{\rho}}\,\frac{1}{\rho-\bar\rho_i}\right]$$

disl-disl.



Considerable change from crack term.

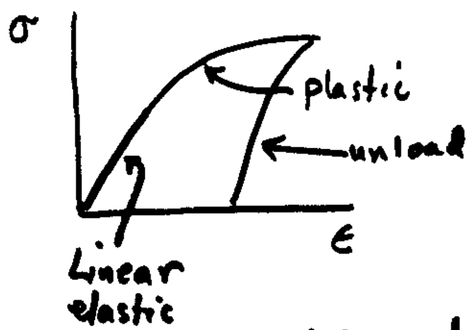


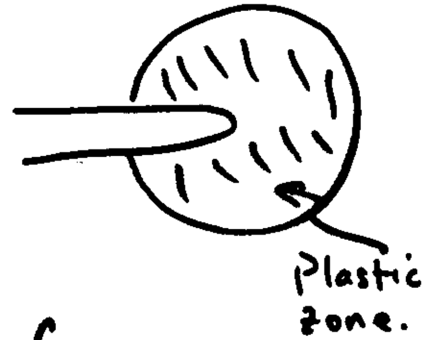
For single crack singularity,

$$f = \frac{k^2}{2\mu}$$

But Eshelby theorem valid for general nonlinear solid.

Known in this form as Rice J-integral





$\sigma(\epsilon)$ a multiple valued fn.
So Eshelby theorem not valid for unload

(Applied any way!)

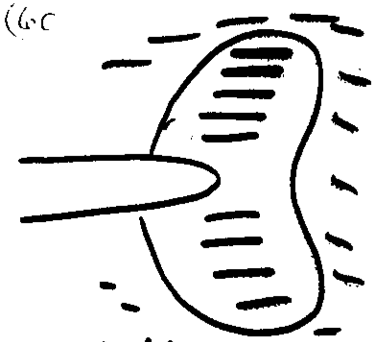
In this way toughness for plastic mat'l.
can be measured using J-ideas —
but not for unload (fatigue)

Idea is that J can be integrated in macro region, + not need to do it thru plastic

Mechanics

Solve elastic-plastic problem from a plastic continuum constitutive law (replaces Hooke's Law)

Highly numerical (finite element)

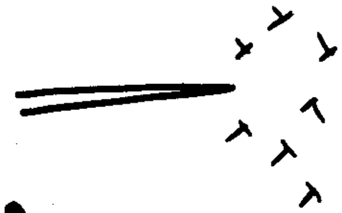


Cannot deal (except empirically) with zone where material physically fails.

Used with considerable success to treat "hole growth" ductile fracture.

Physical

Consider plastic zone to be pure elastic plus dislocations.



Then consider details of crack-dislocation interactions.

Can then hope to deal with close-in zone when disl. # not too large.

Must adopt continuum if large #'s of disl., + revert to mechanics.

J- Integral

(J) $f_k = \int (W\delta_{ik} - \sigma_{ij} u_{j,k})\, ds = \frac{2\pi^2 i}{\mu} \int \sigma^2 dz$

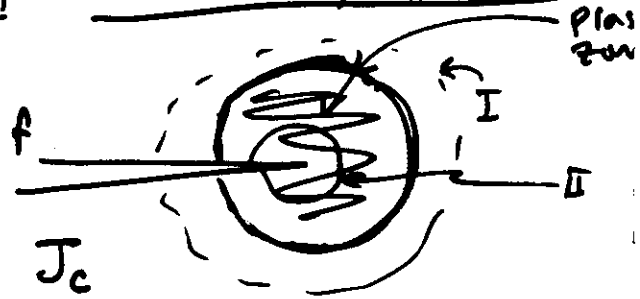
Independent of path by Cauchy theorem

Different Interpretation:

Istead of Hooke's Law,

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

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

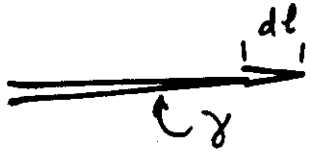


Then J indep. of path, + is a "matl. const". J_c

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

GRIFFITH RELATION

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



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

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 - vali in presence of external chemical environment. So Griffith is a <u>thermo statement</u>, valid under chem. equi

Also limit of kinetics for $v = 0$.

Elastic Overview

1. Cracks + Disl. are singularities in El. fie
2. $\sigma = K/\sqrt{2\pi r}$ 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:

   $f = 0 = f_{elastic} - f_{matl.}$

   γ for crac
   friction str
   for Xloc
6. K gives overall toughness - like J - but contains Xloc. effects.

   (meas. by Narita, et al, Burns, et

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

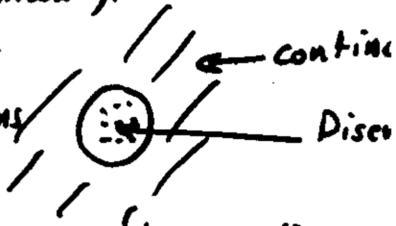
- Stability of crack in lattice (sharp or blunt)
- Chemical Effects at tip – (enhanced reactivity at tip)
- Kinetics of crack motion – (lattice trapping effects.)

Types of Discrete theories

I Classical

1. Inner core with Bondary.

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 Dynamic

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 fits 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 crac phenomena:

1. First Principles Methods.
   Local Density Approx.
      Brute force
      Car-Parinello - optimized to Molecular dynamics

2. Semiempirical
   a. Greens Fn. Expansion - Tight Binding
      1st approx ≡ EAM
      2nd approx → Bending Bond forces.

   b. Embedded atom
      Very simple
      based on embedding energy for an ion in an electron sea.

   c. Cluster molecular calculations of configurations characteristic of solids. (may not be total energy)

3. Lattice (Classical) Calculation
   However a force law is determined, then it is necessary to do a calculation of many atom lattice configuration on basis of Born-Oppenheimer theorem.
   a) Brute force simulation (mol. Dynamics)
   b) Lattice Green's Fns.

Prospect:

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

Crack very complicated extended defect - Pros is for techniques based on valid first principle concepts to be most succes[sful]. Embedded atom good example.

Preliminary Lattice Considerations

Assume the configuration is at equilibrium on the given lattice. Then Excitations give an energy:

$$V = V_0 + \frac{1}{2}\sum_{\substack{ij\\ \ell\ell'}} \varphi_{ij}(\underline{\ell},\underline{\ell}')\, u_i(\underline{\ell})\, u_j(\underline{\ell}') + \cdots$$

If translation (rigid) : v_i

$$\sum \varphi_{ij}(\underline{\ell},\underline{\ell}')\, v_i v_j \equiv 0 \; ; \quad \boxed{\sum_{\ell,\ell'} \varphi_{ij}(\underline{\ell},\underline{\ell}') \equiv 0}$$

Translation by Lattice vector also invariant.

$$\boxed{\varphi_{ij}(\underline{\ell},\underline{\ell}') = \varphi_{ij}(\underline{\ell}-\underline{\ell}')}$$

Invariance wrt rigid rotation of Lattice $\Rightarrow$ zero torque + symmetry of σ_{ij}. (not proven here

Keating Theorem

Invariance wrt Lattice rotation:

$$V'_{Rot} = V$$

V = fn of vector differences:

$$V(\underline{x}_\ell) = V(\underline{x}_\ell - \underline{x}_k) = V(\underline{x}_{\ell k})$$

What kinds of functions of $x_{\ell k}$ are always invariant

Scalar Products of $x_{\ell k}$

Thus

Lattice vectors

$$V(\underline{x}_\ell) = V(\underline{x}_{ik}\cdot\underline{x}_{jk} - \underline{a}_{ik}\cdot\underline{a}_{jk})$$

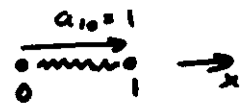
If

$$\lambda_{ijkl} = \underline{x}_{ij}\cdot\underline{x}_{kl} - \underline{a}_{ij}\cdot\underline{a}_{kl}$$

$$V(\underline{x}_\ell) = V(\lambda_{ijkl})$$

Any such fn. will automatically satisfy rotational invariance.

Examples



$$(x_{10}^2 - a_{10}^2)$$

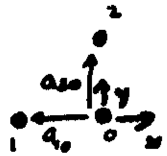
$$= (\underline{a}_{10} + \underline{u}_{10})\cdot(\underline{a}_{10} + \underline{u}_{10}) - a^2$$

$$\cong 2u_{01}$$

$$V = \frac{\alpha}{2}\lambda^2 = \alpha(u_{01})^2$$

Represents simple stretch in spring

2. 3 Body Angular Force:



$$\lambda = (\underline{x}_{10}\cdot\underline{x}_{20} - \underline{a}_{10}\cdot\underline{a}_{20})$$

$$= (\underline{a}_{10} + \underline{u}_{10})\cdot(\underline{a}_{20} + \underline{u}_{20})$$

$$= v_{10} + u_{20}$$

$$V(\lambda) = \beta(\lambda)^2 = \beta(v_{10}^2 + 2v_{10}u_{20} + u_{20}^2)$$

$$f_x\Big]_0 = -\frac{\partial V}{\partial u_0} = 2\beta(u_{20} - v_{10})$$

$$f_y\Big]_0 = -\frac{\partial V}{\partial v_0} = 2\beta(v_{10} - u_{20})$$

3. Non Keating Bending Chains:

$$V = \beta(\theta - \pi)^2$$

(Leads to higher order elasticity. — No Lattice analogue)

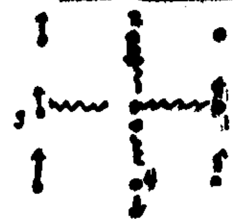
Atoms on Rails

A simple Lattice structure — Non Keat

$$V = \frac{\alpha}{a}(v_{10} - v_{03})^2 + \frac{\beta}{a}(v_{20} - v_{04})^2$$

Bending Bonds (2 body)

Stretching Bonds.



$\underline{u} = u_y$

$u_x = 0.$

This Potential is not invariant to rotation. Depends not only on atom orientation, but also on orientation to underlying lattice. It is thus not a Keating force lattice. and leads to non zero torques. The torques are supplied by "rail constraints".

Nevertheless because of its great simplicity it is a useful 2D model.

Elastic Continuum Limit of Lattices

- Viewed from afar, lattices are continua — How to find this asymptotic relation?

1) Born Long Wave Expansion.
   - Find complete vibration structure with complete dispersion structure
   - Find the $k=0$ limit coincident with $\omega=0$ (acoustic modes)
   - The wave velocities + polarizations for independent modes are expressibl in terms of equivalent sound wa expressions in terms of C_{ijkl}

2) Simpler
   - Expand Keating energy expression $V(\lambda)$. Keep first order derivatives.
   - Separate out "internal strain".
   - Compare with elastic energy density in terms of C_{ijkl}

3) simplest
   - In ~~...~~ simplest cases, find stress + strain analogues.

<u>NB</u> For atoms on rails, elastic limit has non symetric σ_{ij} ! (constraints)

Elastic Limits

<u>Note</u> Cubic continuum 3D
C_{11}, C_{12}, C_{44}

Cubic Lattice
in equilibrium with minimum of
<u>2</u> independent spring constants —
But may have <u>10</u> .... !

Fore example,

In Diamond Lattice
There are only 2 constants which are in dependent.
(there is a relation between C_{11}, C_{12}, C_{44})

For Pair central forces, get Cauchy relations — again only 2 Independe constants.

For long range forces, no elastic measurem can infer more than C_{ijkl} — Some of the bonds do not contribute to macroscopic response

Lattice Green's Fns for Defect Calc.

Force Balance (Statics)

$$\sum \phi_{ij}(\underline{l}-\underline{l}')\,u_j(\underline{l}') = -f_i(\underline{l})$$

(may contain indices for basis atoms.)

$$G = -\underline{\Phi}^{-1} \quad ; \quad u = Gf$$

For perfect lattice,

$$\Phi_{ij}(\underline{l}-\underline{l}') = \sum \Phi_{ij}(\underline{q})\, e^{-i\underline{q}\cdot(\underline{l}-\underline{l}')}$$

$$G_{ij}(\underline{q}) = -\underline{\Phi}^{-1}_{ij} = -\sum_{\text{Shell}} \Phi^{-1}_{ij}(\underline{l})\, e^{i\underline{q}\underline{l}}$$

Shell ↑ finite sum

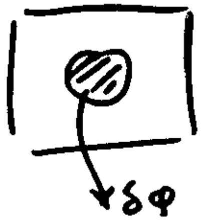
Imperfect Lattice

$$\underline{\Phi} = \Phi^{\circ} - \delta\varphi$$

$$(\underline{\Phi}^{\circ} - \delta\phi)G = -\mathbb{1}$$

$$G + G^{\circ}\delta\varphi G = G^{\circ}$$

$\delta\varphi$ projects this eqn onto finite space (defect space)



Order of matrix

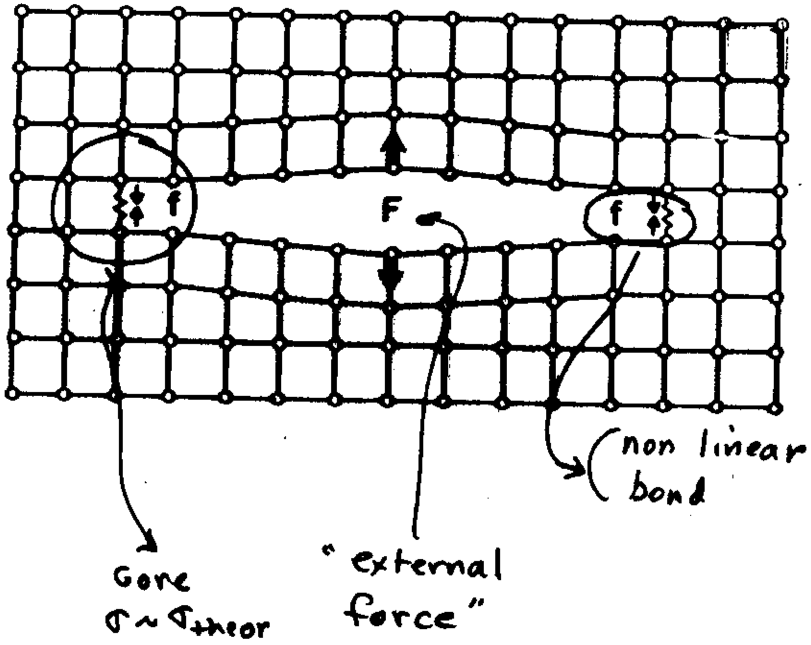
$(nL)^3$ 3D

$(nL)^2$ 2D

$L =$ size

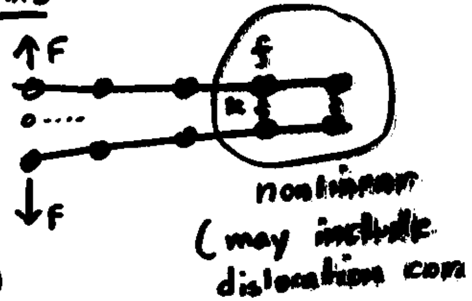
$n =$ 1-6

Schematic Model of a Crack



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

Nonlinear Problems



$u = GF$

$$\begin{cases} u_0 = g_{00}F + \Sigma\, g_{0k} f_k(u_k) \\ u_k = g_{k0}F + \Sigma\, g_{kk'} f_{k'}(u_{k'}) \end{cases}$$

A small set of self consistent eqns. to be solved (relaxation) (Esterling

(Note difference with Mol. Dynamics - G gives response of entire lattice to each iteration of non linear bond.)

Why Green's Fns?

1. Requires Reference Lattice
2. Static (quasi static!)
3. Solves LARGE problems. $\sqrt{10^7/p}$ atoms in Defect Space
4. Asymptotic relations available for larger problems.
5. periodicity helps.

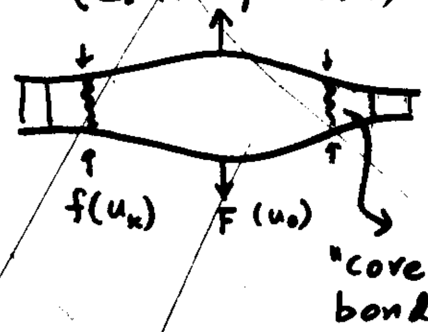
Examples

Entire array of atomic Problems at crack tips.
- Interfacial cracking + Disl. Emission
- Chemical Interactions at Cracks.
- 3D crack Problems.
  - kink formation during Chemical attack (Act. barriers)
  - Bridging of cracks by Random hard spots

Non Linear Bonding Paradigm

(Esterling, 1976)

Green's fn. Master Eqn.:



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

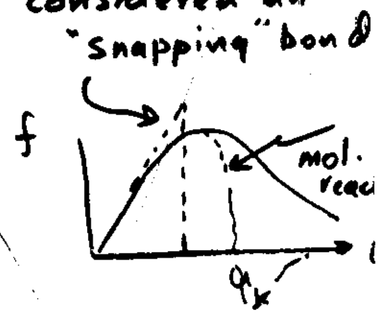
$$u_k = g_{k0}F - \Sigma\, g_{kk'} f$$
$$= g_{k0}F - g_{kT} f$$

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

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

Actually

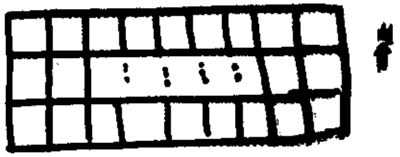
$$f = f(u_k)$$



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

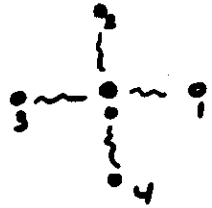
This represents the real power of Green's

Simplest Lattice Crack (Lattice on nails)



$$V = \sum \frac{\alpha}{2}(v_{10} - v_{02})^2 + \frac{\beta}{2}(v_{20} - v_{04})^2$$

↑ Bending ↑ Stretching



$$\phi = \frac{\partial^2 V}{\partial v_l \partial v_{l'}}$$

$$\sum \phi(l - l')\, u(l') = F(l)$$

$$\varphi(0, j) = \begin{bmatrix} -2(\alpha+\beta) & ; \beta & ; \alpha & ; \beta & ; \alpha \end{bmatrix}$$

$\varphi(00)$ $\varphi(10)$ (20) (30) (40)

Fourier Expansion

$$\varphi(q) = \frac{1}{2\pi}\sum \varphi(l)\, e^{-iq\cdot l}$$

$$= -\frac{1}{\pi}\left(\alpha \sin^2\frac{q_x}{2} + \beta \sin^2\frac{q_y}{2}\right)$$

$$G(q) = \frac{-\pi}{\alpha \sin^2\frac{q_x}{2} + \beta \sin^2\frac{q_y}{2}}$$

$$\boxed{G(l) = \frac{1}{2}\iint_{-\pi}^{\pi} \frac{e^{iq\cdot l}}{\alpha \sin^2\frac{q_x}{2} + \beta \sin^2\frac{q_y}{2}}\, dq_x\, dq_y}$$

can do one integral by complex varia
(integrate over unit circle)

Cont

But $G(l)$ Divergent!

$G(q)$ divergent at origin. (logarithmic divergence)

Two options:

1) Define Dipole G:

$$\varphi G = D(l)$$

$$G(q) = \frac{-\pi\left(1 - e^{-iq_y}\right)}{\alpha \sin^2\frac{q_x}{2} + \beta \sin^2\frac{q_y}{2}}$$

2) Always take forces which balance.

Then divergence for F^+ balances F^-.

Dyson Eqn

From Symmetry $G(l_x, \tfrac{1}{2}) = G(l_x, -\tfrac{1}{2})$

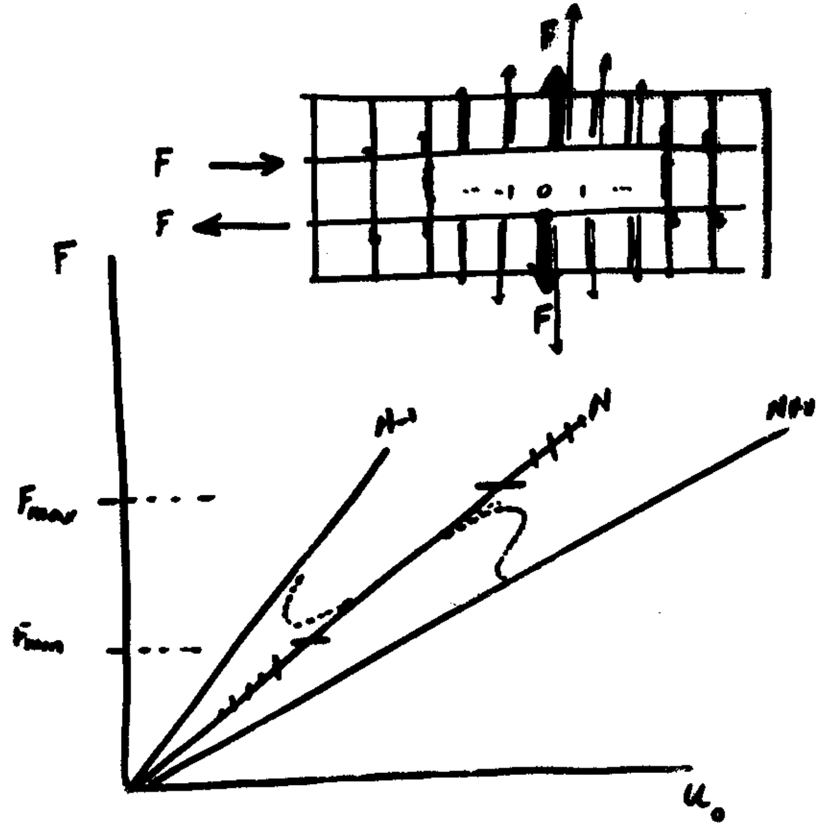
$$\delta\varphi(l_x, \tfrac{1}{2}; l_x', \tfrac{1}{2}) = -\delta\varphi(l_x, \tfrac{1}{2}; l_x', -\tfrac{1}{2}) = -\beta\,\delta_{l_x; l}$$

$$\sum_{\substack{l_x'' \\ \text{crack}}} \left[\delta_{l_x, l_x''} - 2\beta\, g_0(l_x; l_x'')\right] g(l_x''; l_x') = g_0(l_x; l$$

assume Dipole force here for g_0

This is a matrix eqn. of rank = l_k. (crack length

LATTICE RESPONSE Fn Diagram

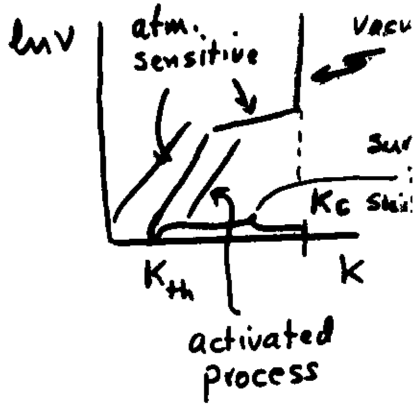


$$u_0 = g_{00} F = g_{00}(N) F$$

$$\left[\begin{aligned} u_0 &= g_{00} F + g_{0N} f(u_N) \\ u_N &= g_{N0} F + g_{NN} f(u_N) \end{aligned}\right]$$

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 reacti[on]

Must study local fluctuations (3D) in crack config. induced by chemica[l] reactions at local site.

a) Small molecules: Reaction at tip bond

b) Large molecule: Penetration into crack mouth restricted.

- What is criterion for penetratio[n]
- What mechanisms exist for growth for no penetration?

Reaction Paths for Small Molecules

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

Thus require general theory of crack structure required:

Paradigm

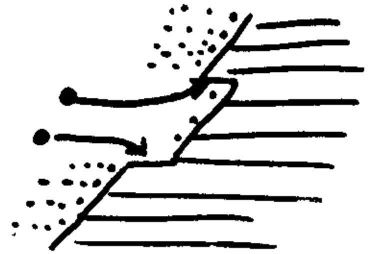
1. Develop a Green's fn. formalism for linear Cracked lattice
2. Put in non linear bonds.
3. Calculate reaction path, + $E_{act.}$ (kinked crack)
4. Include external chemical species
5. Entire procedure assumes knowledge of force laws.

Plan of Attack

1. Small molecules: penetration assured,

Assume molecule attacks crack tip bond.

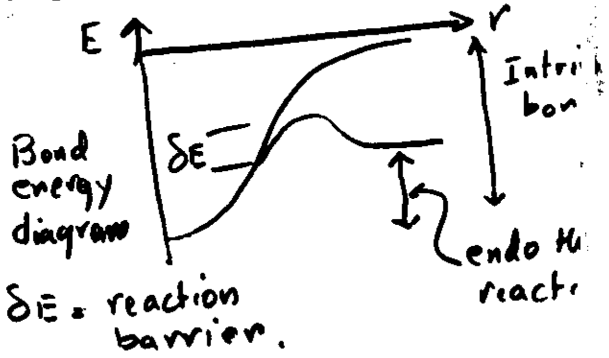
After reaction, surface is covered $\gamma_0 \rightarrow \gamma_1$ in Griffith rel



Crack growth is by nucleation + Growth of kink pairs on crack

How do barriers arise ??

1. Atomicity: Lattice trappi
2. chemical reaction barri

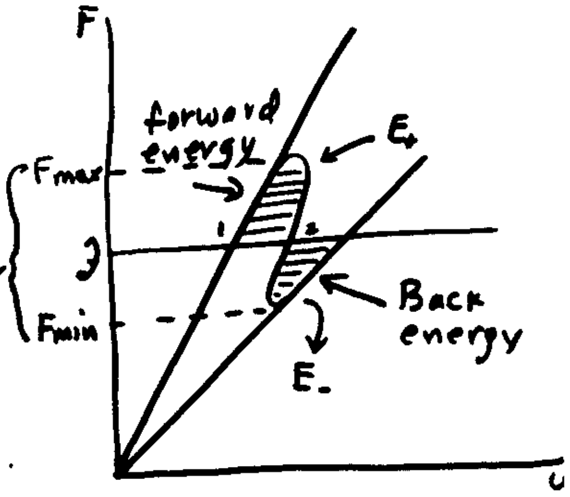


Energy Barriers

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

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

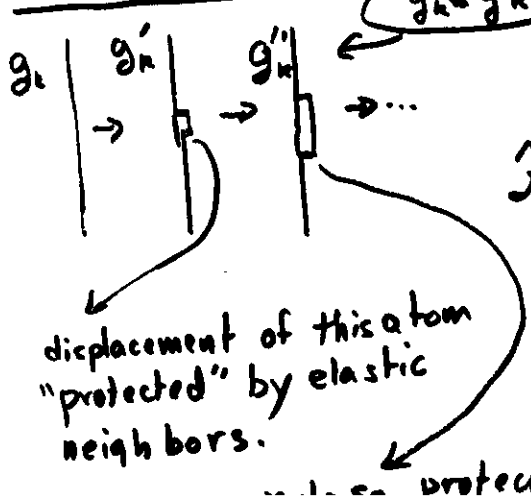
trapping range (mechanical stable)

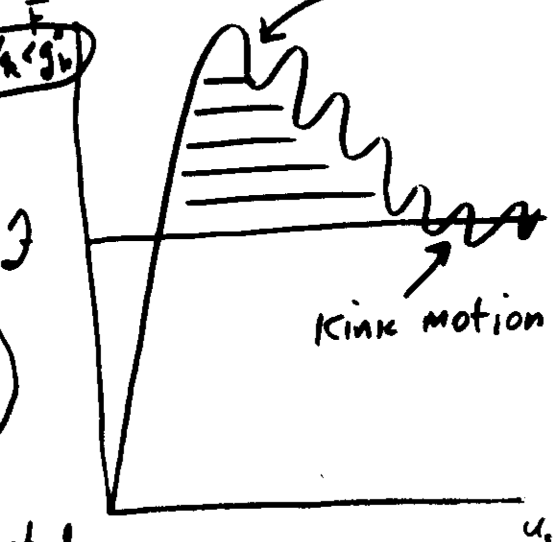


$\mathfrak{F}_{Griffith}$: $E_+ \simeq E_-$

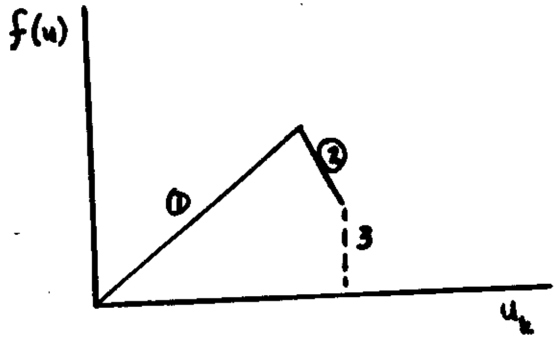
valid for kink motion energy, or for 2D crack motion.

Kink Nucleation:

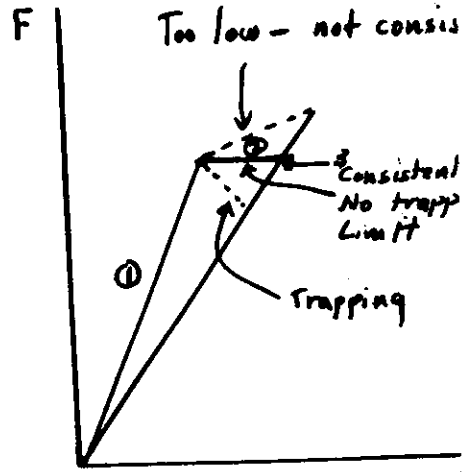




One Atom Core Criterion



Self consistent force law for limiting response function.



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

From Greens fns Master Eqn.

$$du_k = g_{k0}\,dF - g_{kr}\,df \qquad (dF=0)$$

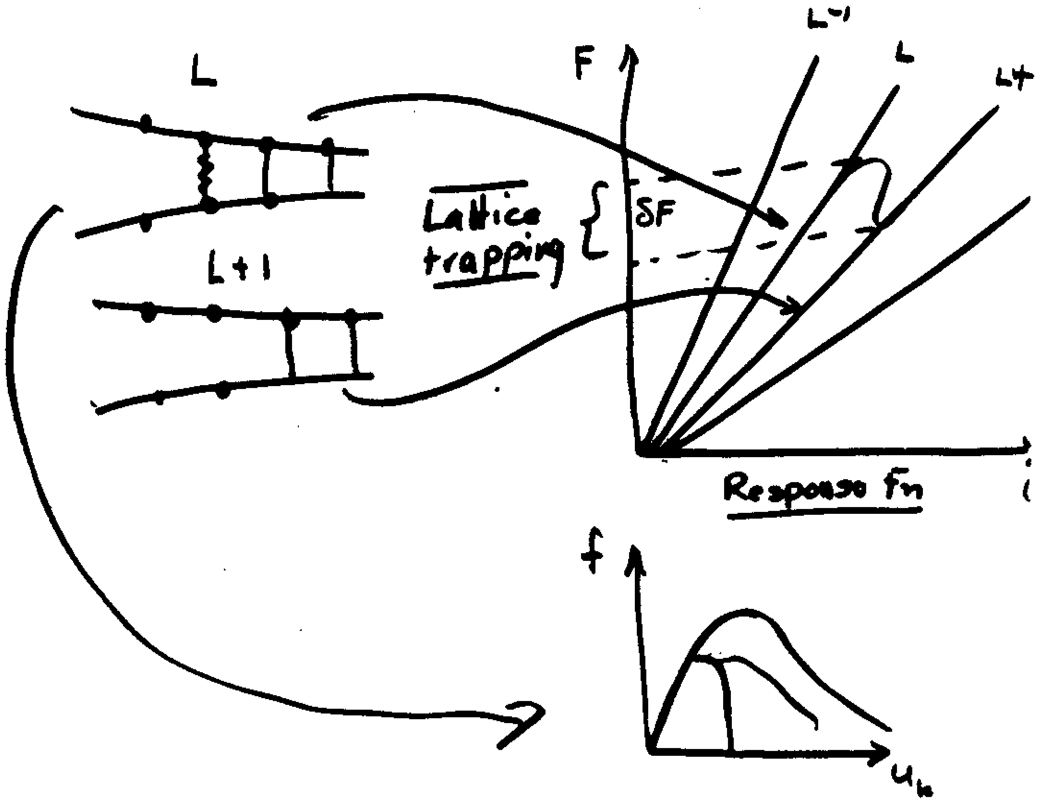
$$\boxed{\left.\frac{df}{du_k}\right|_{\text{back side}} < -\frac{1}{g_{kr}} = -\frac{B}{h_{kr}}}$$

← elastic modulus

← number (dimens

- For trapping to be observable, force law must be almost snapping. Thus, no trapping for ... 1 atm required — specia

CRACK RESPONSE FNS + GRAPHICAL ANALYSIS



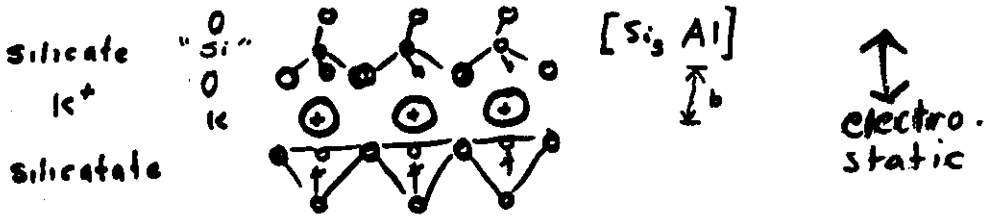
As tip bond goes nonlinear + breaks, response fn. goes from $L \to L+1$, with nonlinear excursion between $F(u_0)$ lines.

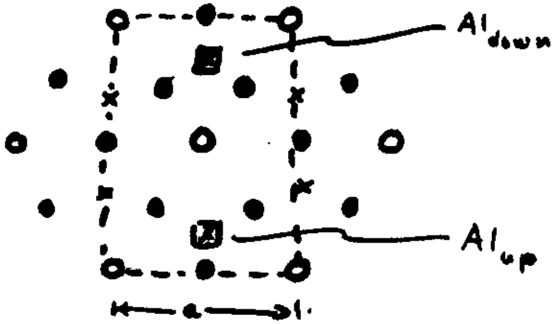
Over lattice trapping range, crack does not change length. This results in energy barriers.

Molecular Wedging in Chemically Enhanced Fracture

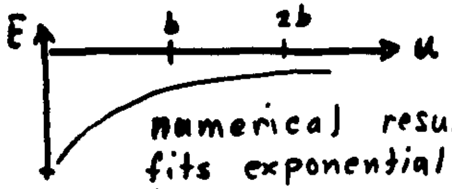
1. General idea — D_2O molecules penetrat
2. Mica - Water Force Laws
3. Green's Fn. Analysis of Wedging (dis
4. Conclusions
   - a) Detailed analysis required
   - b) Shape of crack modified
   - c) Molecular wedge region created
   - d) Transport thru wedge important

Mica/~~water~~ Bonding





1. primary bonding in silicate is covalent
   Al serves as substitutional donor.
2. Electrostatic Energy



numerical result fits exponential law.
$\delta c = 0$.

$$E_{vac} = A e^{-\alpha u} - B e^{-\beta u}$$

$$= .59 e^{-21.5 v} - 3.6 e^{-3.33 v}$$

(ev)

Fit: electrostatic energy, lattice const, elastic c

γ_{vac}.

Water Interactions

1. One layer. Expands K layer ~ 50%
   treat water as dipole.

$[\delta V]_{H_2O} = 1.6$ ev.

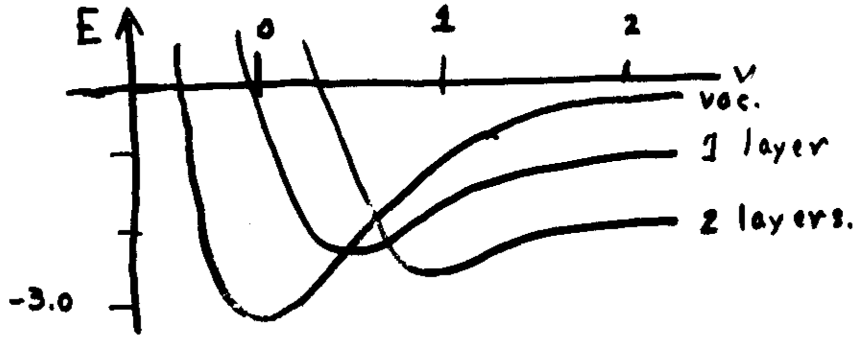
$$E_1 = 1.19 e^{-10.75(v-.170)} - 3.6 e^{-3.33 v} - 1.6$$

2. 2nd Layer. Further expansion to .6

$[\delta V]_{H_2O} \cong 2.0$ ev

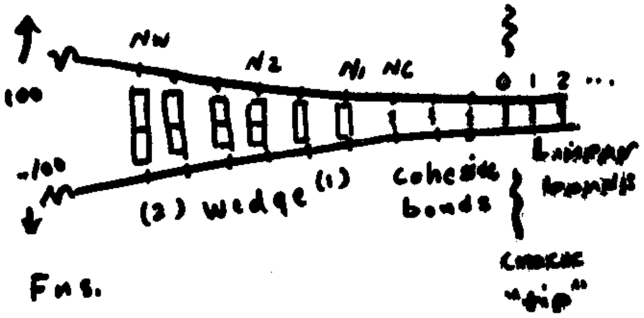
$$E_2 = 1.77 e^{-7.17(v-.318)} - 3.6 e^{-3.33 v} - 2.0$$

Total Potential



2D CRACK PROBLEM

Lattice is tetragonal
(convert Mica to "effective" tetrahed.)



1. Find Lattice Green's Fns. for Lattice

2. Assume nonlinear bonding + wedging to left of tip consistent with Energy fn.

Solve

$$v(l) = F_0\, g(l, -100) + \sum_{l'=1}^{NW} f(v(l'))\, g(l; l')$$

3. Nonlinear in TWO ways!
   a) force law, $f(v(l'))$ is nonlinear
   b) Positions of wedge tips not known

Note: By defining First linear bond, problem is always (almost) well ~~def~~ posed for mechanical equilibrium.

Note: K fields + linear Fract. Mechanics ideas not valid when N_1, N_2 small.

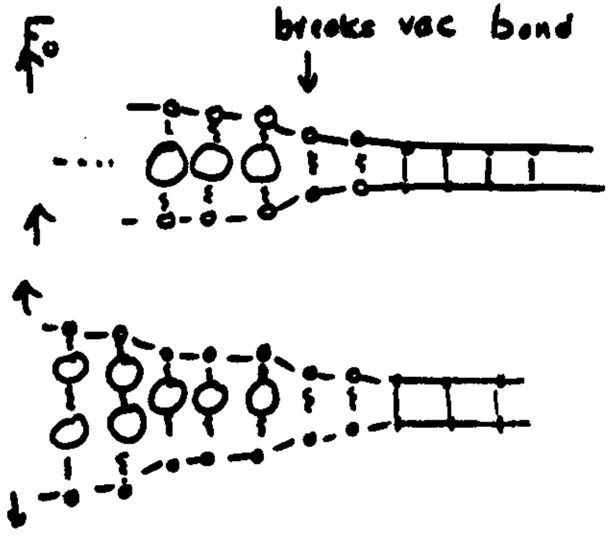
Note: No problem with Barenblatt Subtleties — never any singularities

Results

Load: F_0 at Threshold!

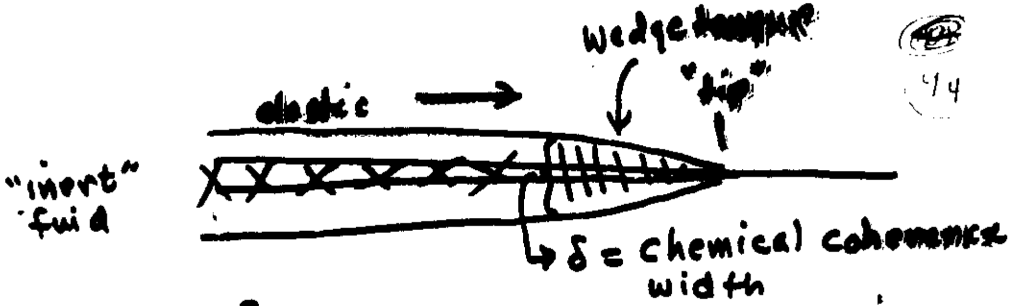
1st Stage
1 layer
Full penetration

2nd Stage
2 layers.



Physical Description

1. For one layer, mica wraps around wedge tip — sudden bond breaking.
2. 2nd layer can find mechanical stability nearly any where!
3. Stationary Config:
   Mechanical work to move 2d layer one lattice spacing
   = electrostatic (chemical) energy gai
4. A wedge "tongue" develops at crack tip



Conclusion

Crack growth barriers:

1. Chemical + lattice trapping barriers at tip
2. transport through wedge tongue

[3. Regrowth very rate dependent (# entrapped layers is rate dependent)

Green's Fns Summary

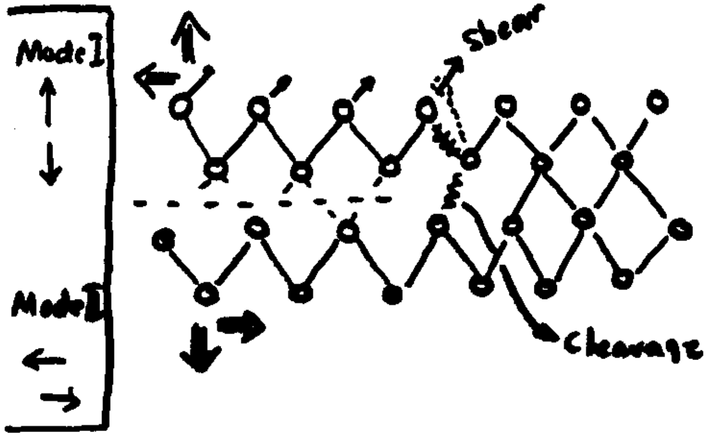
- Excellent method for exploring barriers to crack growth with external chemical environment.
- Important to develop criterion for penetra:
- Crack growth by chemical reaction at tip only possible for reaction paths of "snapping" character.
- Kink formation energies in SiO_2 ≤ 2 ev motion energy ~ 0.1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

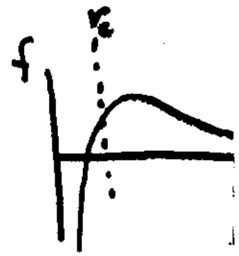
Fundamental Criterion for Ductility

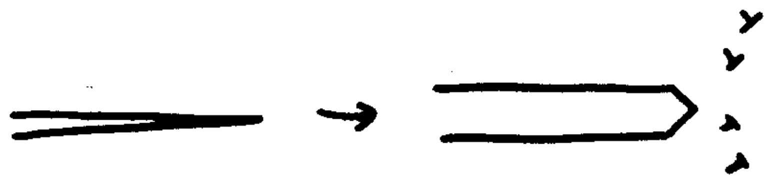
- Intrinsic Ductility
  Disl. emission + Crack Stability.
- Extrinsic Ductility (Ductile Xtion)
  Inhomogeneous crack sources
  External sources.

Intrinsic Ductility

Is a Brittle Crack Stable?







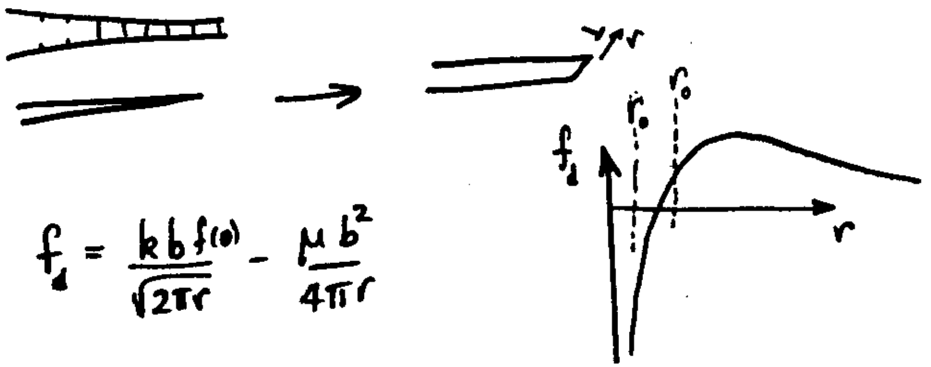
- If emission (shear failure) occurs before cleava[ge]
  no brittle crack is stable in lattice.
  (Blunted crack cannot cleave!)

Criterion Depends on
- character of bonding
- mode of loading
- Chemical attack at crack tip
- interfacial crack
- crystallography

} Really a[n] atomic Propert[y]!

Atomic calculations by
Kaxinen, Markworth, Sinclair, Argon + Yip,
Dienes, Paskin, Sieradzky. Esterling, Baskes, Daw. / R[...]

I Dislocation Emission (Athermal) 2D



$$f_d = \frac{k b f(\theta)}{\sqrt{2\pi r}} - \frac{\mu b^2}{4\pi r}$$

$$\begin{cases} k_e = \dfrac{\mu b}{2\sqrt{2\pi r_0}} \\ k_c = 2\sqrt{\mu^* \gamma} \end{cases}$$

$$\boxed{k_e \gtrless k_c}$$

Stability Parameter

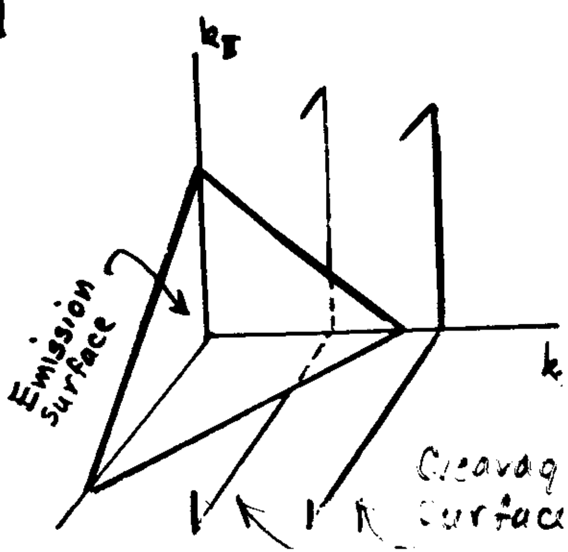
$\beta = \sqrt{\frac{\mu b}{\gamma}}$ $\quad \beta_{crit} \sim 3$

also r_0; xtallogr.

In Mixed Mode

$$f_d = f_d(k_I, k_{II}, k_{III})$$

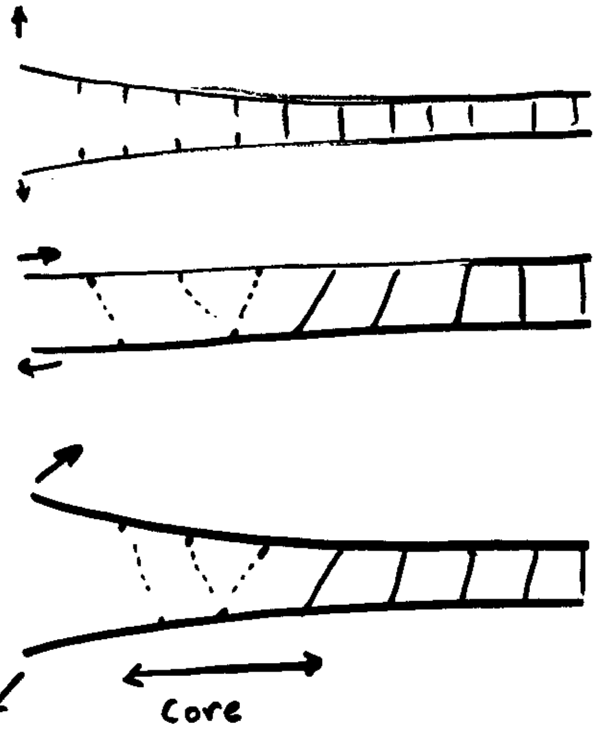
$$k_c = k_c(k_I)$$



Cleavage

$$k_I^2 = \frac{4\mu}{1-\nu}\gamma \qquad \text{Griffith}$$

Dependence on k_{II}, k_{III}?



Core of crack >> core of xloc. but separation of crack must occur within core distance for xloc. Thus mode II does not help.

Genl Predictions

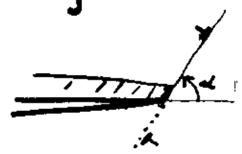
1) Solid Types

- fcc Metals emit before cleave
- bcc Metals cleave before emit (Fe ?)
- NaCl cleave
- Diamond cleave.

— Dynamic.

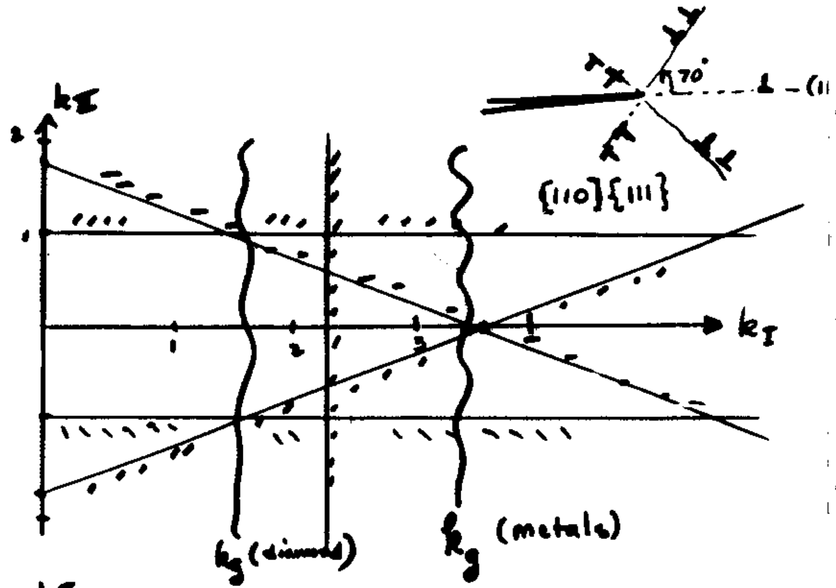
In mixed mode, emission criterion

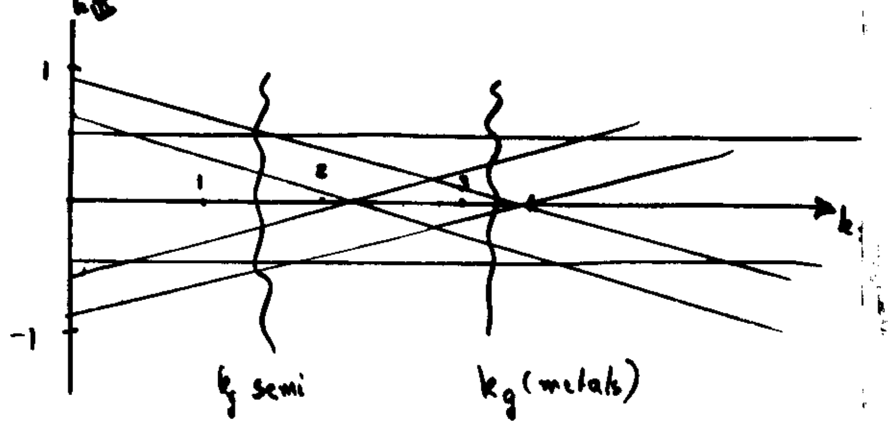
$$b_s k_{IIIe} f_3(\alpha) + b_e \left[k_{Ie} f_1(\alpha) + k_{IIe} f_2(\alpha) \right] = \frac{\mu}{2\sqrt{2\pi r_0}} \left(b_s^2 + \frac{b_e^2}{1-\nu} \right)$$



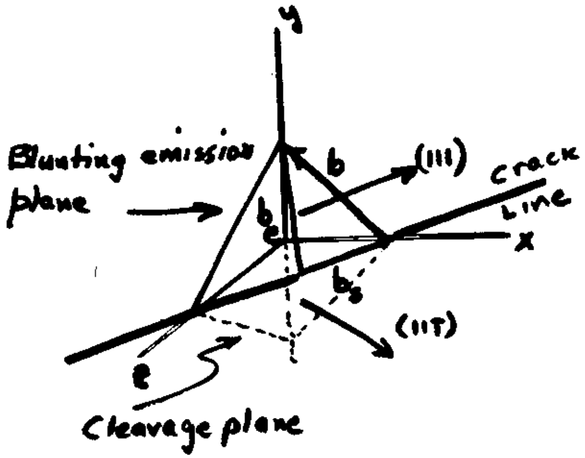
$b_e = \frac{\sqrt{3}}{2} \quad b_s = \frac{1}{2}$

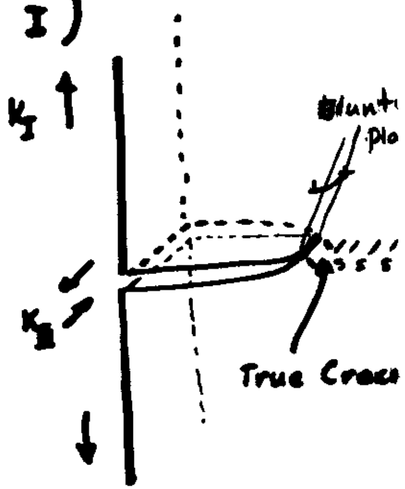
- FCC



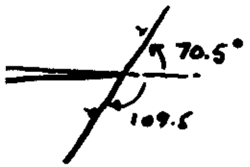


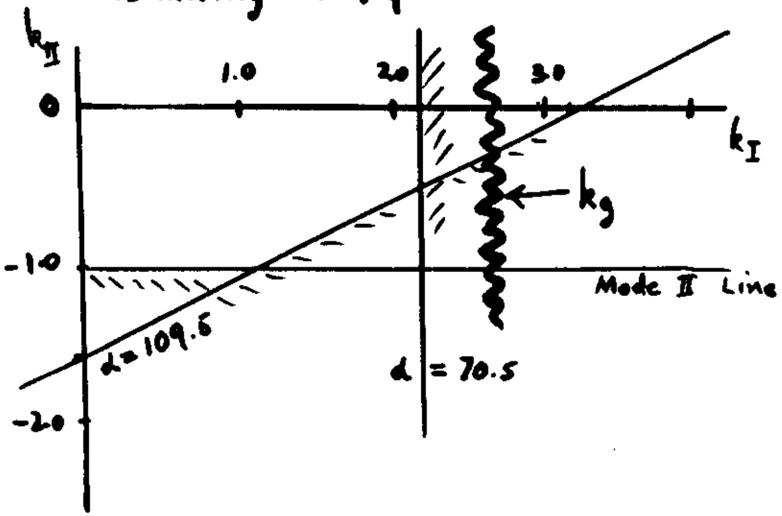
Ohr Configuration (Case I)





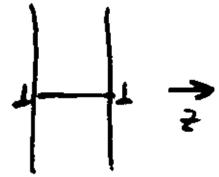
Stability Diagram (k_I/k_{II} cut)
Blunting Config





This material never cleaves!

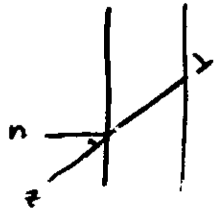
Long Range Stresses in Foils
(No buckling)



$$\sigma_{ij} \cdot n_j = 0$$

$$\sigma_{zx} = \sigma_{zy} = 0$$

For screw $\sigma \sim e^{-r/d}$

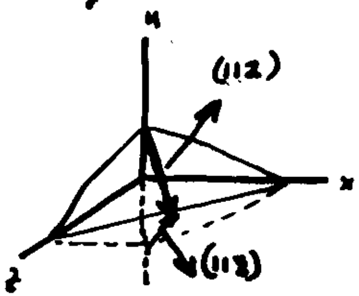


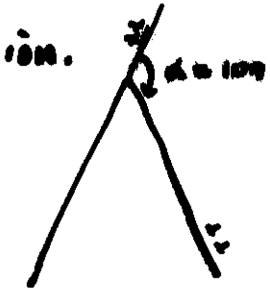
$$\left.\begin{aligned} F_1 &= \sigma^{\infty}_{13}\, n_3 \\ F_2 &= \sigma^{\infty}_{23}\, n_3 \\ F_3 &= \sigma^{\infty}_{31}\, n_1 \end{aligned}\right\}\ \text{partial Cancell.}$$

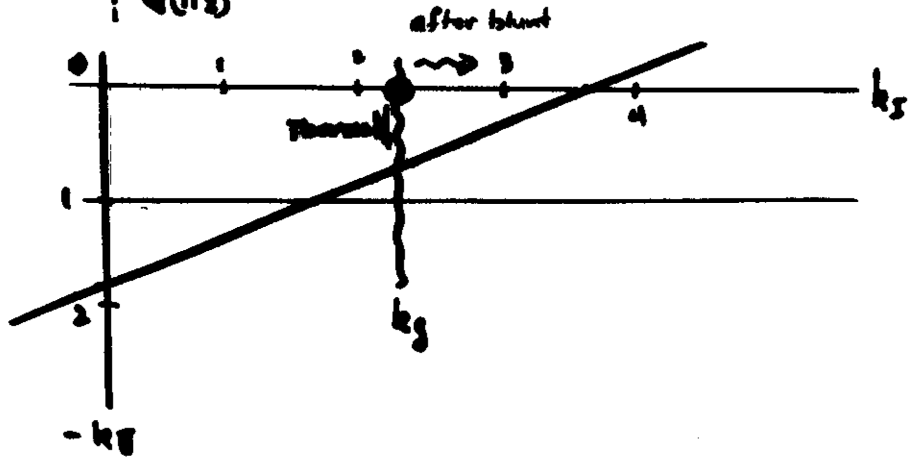
For $r \gg d$ $\quad \sigma^{s}_{32} \sim \sigma^{\infty}_{32}\, n_3$

forces on xloc $\sim f^{\infty} n_3$

Mode I/II Serrated Configuration.







<u>Branching</u> <u>Condition</u>

$$K_I^{Br} = .19206\ k_I + .81652\ k_{II}$$

Mode mixing

$$\frac{K_I}{K_{II}} = .353$$

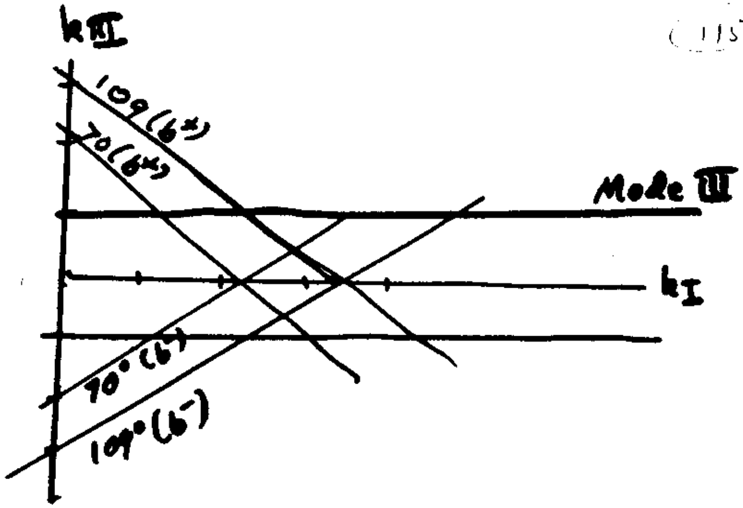
$$\frac{\Delta K^{Br}}{\Delta K_{ext}} = .3$$

$$\frac{\Delta K^{OLD}}{\Delta K_{ext}} = .1$$

<u>BRANCHING</u> <u>AFTER</u> <u>BLUNT.</u>

k/k_{III}

ut



Conclusions

There exist no regime for cleavage
for shear cracks

Mike's cracks must be blunted
so it can sustain $k_I < k_{Ig}$

Extrinsic Plasticity Major Questions

1. what is Role of antishielding?

2. what are prospects for external plasticity to produce a ductile (tough) material?

   If sources every where, μ_D large. Yes

   But [Sources are widely scattered
   $\mu_D(T)$

3. Mathematics

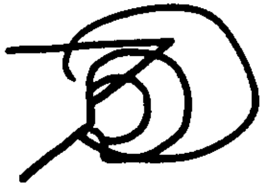
   Many Body
   Long range Interactions $\frac{1}{\sqrt{r}}$, $\frac{1}{r}$
   3D!

Extrinsic Ductility

(Ductile/Brittle Transitions)

Two Types of Transition

No external Sources (Si)



Ledges can make dislocati... (inhomogeneous sources on crack verified by Bu...

External Sources (Plastic~~ity~~ Polarization)

$\sum b_i \equiv 0$

Stress intensity factor

$$\sigma = \frac{k}{\sqrt{2\pi r}} f(\theta)$$

If K is measured stress intensity (macroscopic)

$$K = k + \sum_D k_i^D(b)$$

↑ determined by atomic considerations

$$k_i^D \propto \frac{b_i}{\sqrt{2\pi r_d}}\, g(\theta) \rightarrow \boxed{\text{has sign of } b}$$

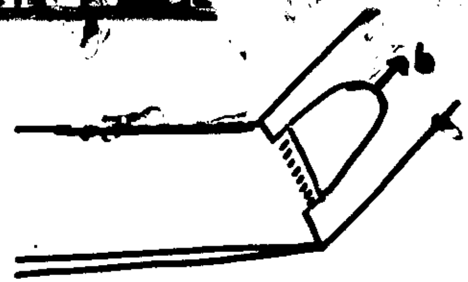
i.e. shielding or antishielding

Emission Nucleation (3D) (ELASTIC Continuum)

SLIP PLANE INTERSECTS CRACK

BLUNTING

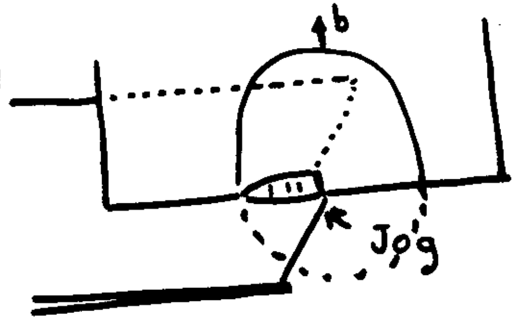
K_I config



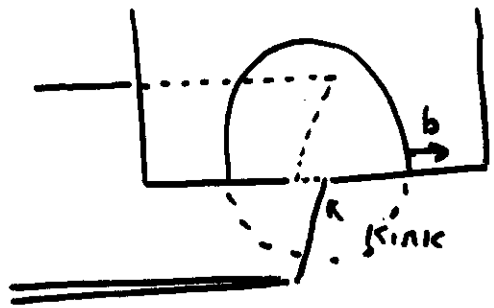
K_{II}, K_{III} config

SLIP PLANE DOES NOT INTERSECT CRACK LINE

Jog Config



Kink Config



ucleation Energy

Early suggestion :

$$E \gtrsim 10\,\text{ev}$$

Now

$$E_{\text{blunt}} \simeq 0.5\,\text{ev} \quad \text{in Si}$$

Simple Estimate for Jog (kink) :

$$E_{\text{blunt}} \simeq \frac{1}{2} E_{\substack{\text{Jog}\\ \text{kink}}}$$

(does not include good estimate of image, optimum shape - etc.)

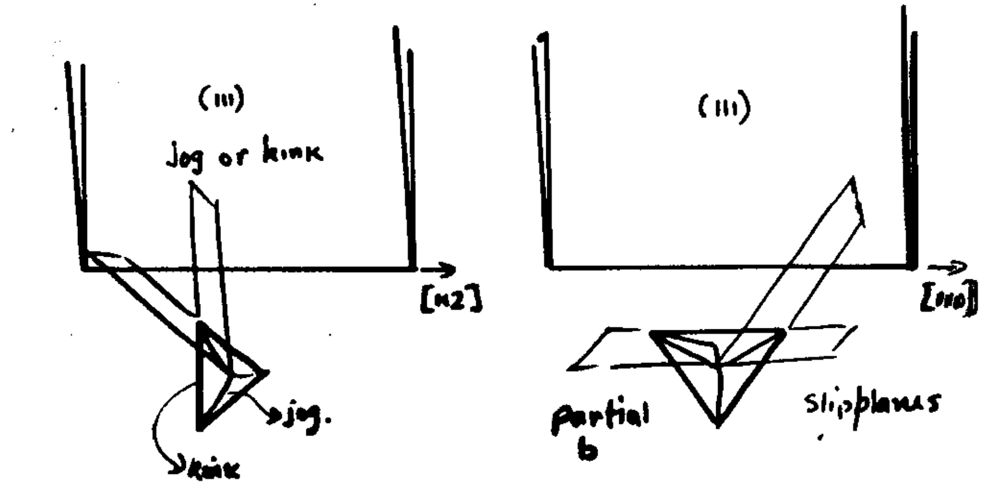
Summary

Experimental studies of Emission
Mostly Brittle Matls.

Author	$k_e^{meas}/k_e^{th.}$	Comments		
Ohr etal	~ 1	Thin foils - Metals - DFZ.		Mode III
Burns etal	$\ll 1$	Inhomogeneous	Etch pit; LiF	Liga
Michot	$\ll 1$	Inhomo. $E = E_m$	Si/Etch pit Jog/Kink preferred	Ligamen
Haasen/Seeke	$\ll 1$	$E = E_m$	Si/etch pit	Ligamen
Hirsch, Roberts, etal	$\ll 1$	Inhomogeneous (Indentation) $E = E_m$	Si/Etch Small crack	Ligamen
Hockey	?	Inhomogeneous	Si/Al_2O_3 MgO / TEM	Ligament (special sites)
Gerberich	$\ll 1$		NaCl/Blunt preferred	
Clarke etal		Homogeneous (?) (silicon)	Exact low. hi res TEM	

Sharp BDT

Silicon (A brittle matl which emits easily)



Experimental

Hockey	Chiao Clarke	Brede Haasen	Michot	Hirsch et al
Jogs (?)	Jogs Mode III	Jogs	Jogs + Kinks	Blunt (extrinsic)
el M.	el M.	x ray etch.	X ray	el M.

~~Theory~~

~~Blunting vs. jogs+kinks~~

~~E_{act} (S.F, Image, shape)~~

~~Mode II ?~~

~~Suggests emission not hard (Genl) (Argon)~~

Narita, et al.
Scripta Met. 21 1273

Anti shielding Dipoles circled

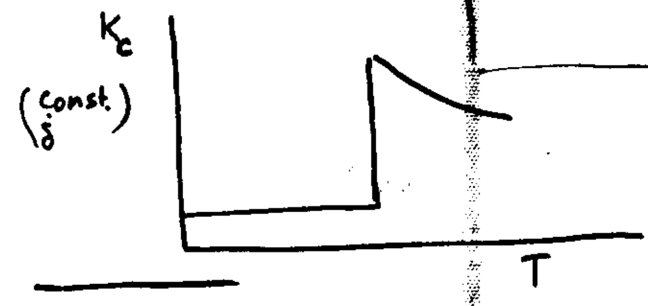
Shielding accomplished early – then dipole formation + saturation.

#	Δk_{IC}	k^D
620	.1	.13
2000	.09	.32
3000	.05	.45

(MPa $\sqrt{m}$)

Analysis by Zhou et al

Silicon



Experiments suggest shielding unstable + saturates.

Fig. 2

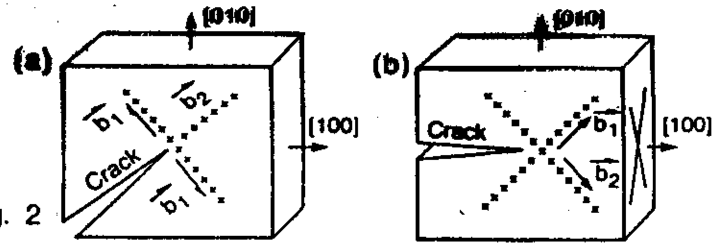


Figure 2. A schematic representation of (a) ($\bar{1}10$) plane crack with (110) and ($\bar{1}10$) plane edge dislocations. (b) (010) plane crack with (110) and ($\bar{1}10$) plane edge dislocations. The more common screw dislocations are lightly shown on the (100) face.

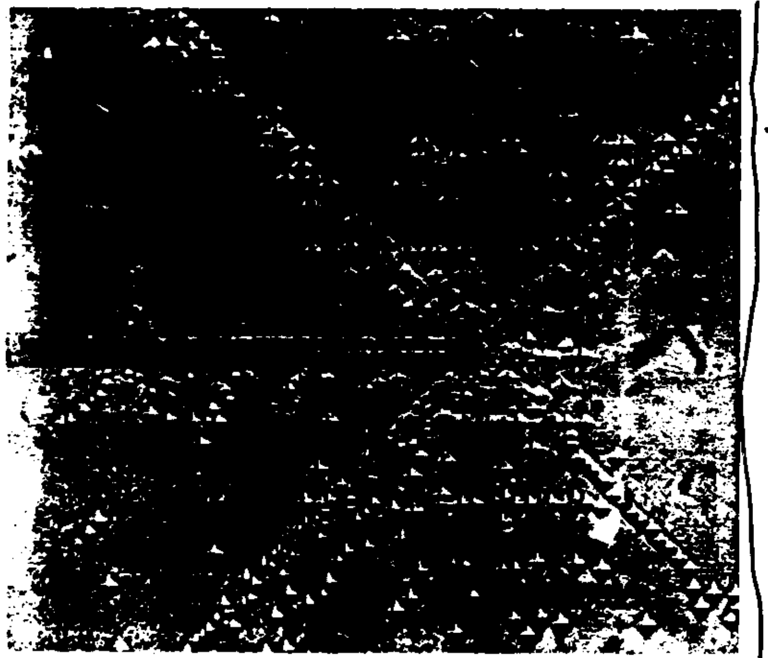


Figure 3. A photomicrograph of crack tip deformation in 2(b). The horizontal line is the crack. The cross are edge dislocations, some screw dislocations are also seen parallel to the crack.

Also Fu et al

Zn

$k_e^{II} \ll$ Theo

k_e is k^I

Ohr

$k_e \approx$ Theo

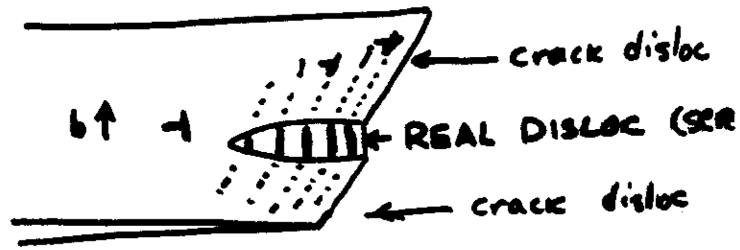
Burns, Scripta Met. 20 1489 1986

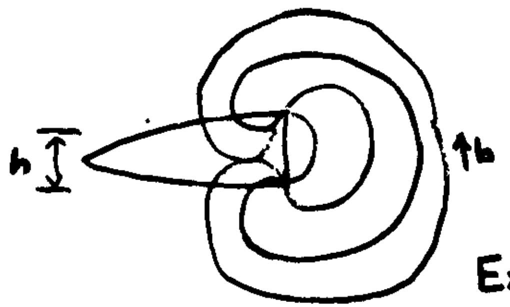
Very small k_e based on measured shielding (?) (dipoles ?)

What Are the Inhomogeneous Sources?

1. Hirsch et al Model
   emphasis on crack/disl source

2. Flat Cracks in Large Specimens
   Ligament Model. (Jog configuration)



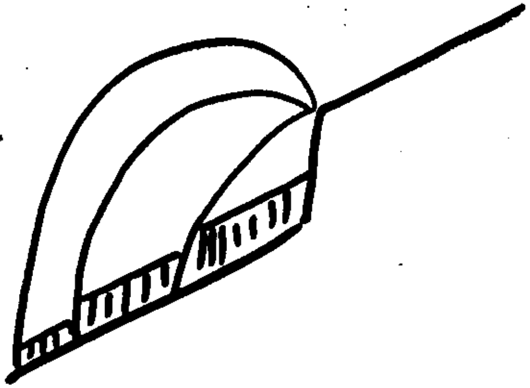


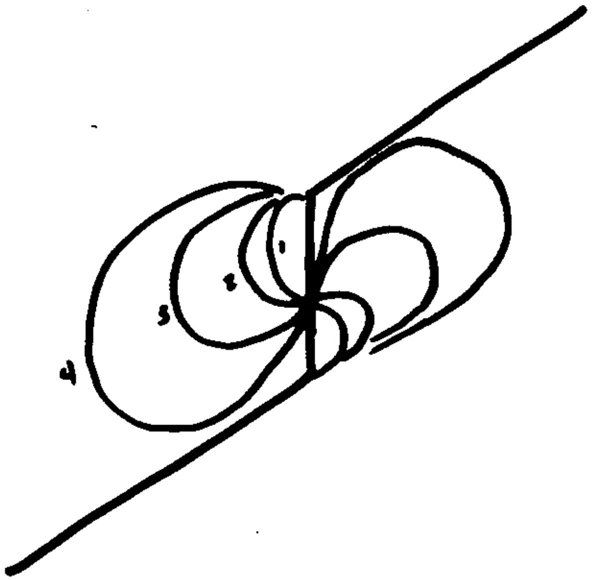
Exhaustion Source.

$$k_e \sim \frac{\mu b\, f(\theta)}{\sqrt{h}}$$

$N = h$

Blunting Configuration

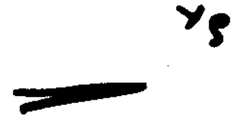




Again, Source exhausted when ligament is used up.

External Sources & Dislocation Shielding

Ashby et al



Mode III

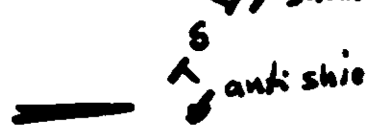
$$\sigma(x,y) = \sigma(z) = \sigma_{32} + i\,\sigma_{31}$$

$$= \frac{K}{\sqrt{2\pi z}} + \frac{\mu b}{4\pi}\left\{ \frac{1}{z-\xi}\left(\sqrt{\frac{\xi}{z}}+1\right) + \frac{1}{z-\bar{\xi}}\left(\sqrt{\frac{\bar{\xi}}{z}}-1\right)\right\}$$

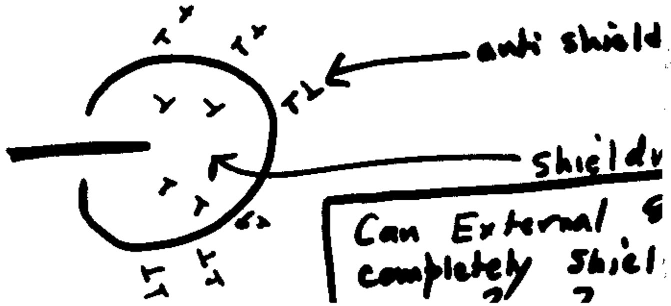
applied K · sign of b · free field term · contribution to K · image

$$k = K - \frac{\mu b}{2}\left(\frac{1}{\sqrt{2\pi\xi}} + \frac{1}{\sqrt{2\pi\bar{\xi}}}\right)$$

Force on dislocations + cracks given by residues of σ at defect



Narita et al
Experiments



Can External S
completely Shiel
?

II Dislocation Shielding

[external sources
emitted Xloc.]

Any source of internal stress at the crack tip will load the crack + create $k^{(shield)}$

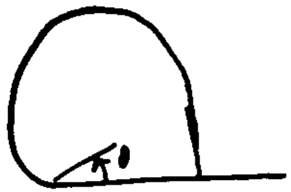
Screw Dislocation

$$k^D = \frac{\mu b}{2\sqrt{2\pi}}\left[\frac{1}{\sqrt{\xi}} + \frac{1}{\sqrt{\bar{\xi}}}\right]$$

edge more complicated.

k^D_{II}
(b_x)

k^D_{I}
(b_y)

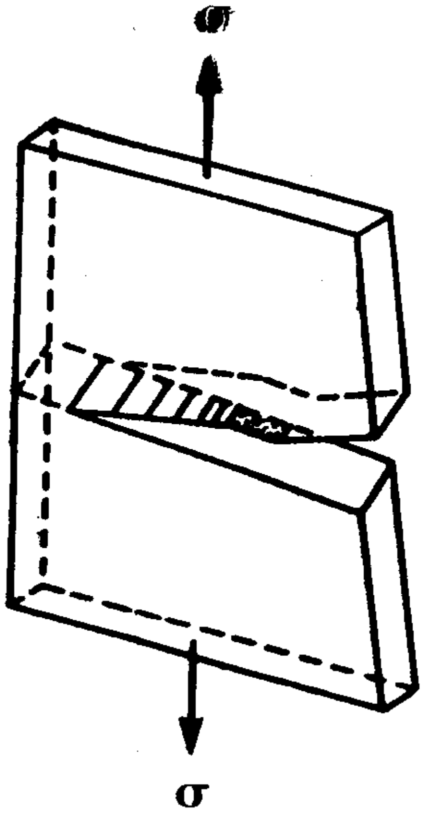


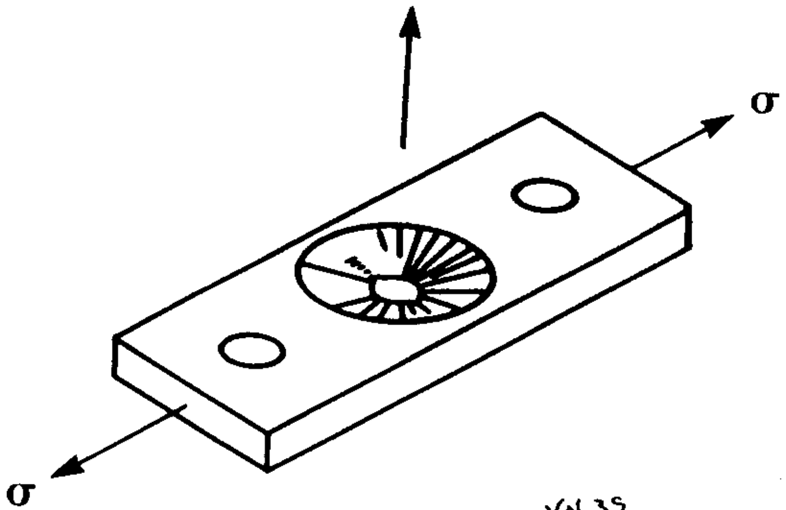
Shielding Matrix

	I'_y	I	II	III
k^D_I	+	+	0	0
k^D_{II}	±	0	+	0
k^D_{III}	0	0	0	+

"orthogonality" of Modes.

(129)





-SSP-1 Vol.39 12 45

(130

BOUNDARY	θ /[H K L]	SYSTEM	$\Delta\theta$ / $\Delta\theta_{max}$
Boundary 1-2:	46.64°/[9 8 6]	—	—
Boundary 1-3:	9.76°/[2 1 1]	—	—
Boundary 2-3:	57.00°/[4 4 3]	Σ 3, 60.00°/[1 1 1]	0.95

Fig. 1. Intergranular crack meets a triple point.

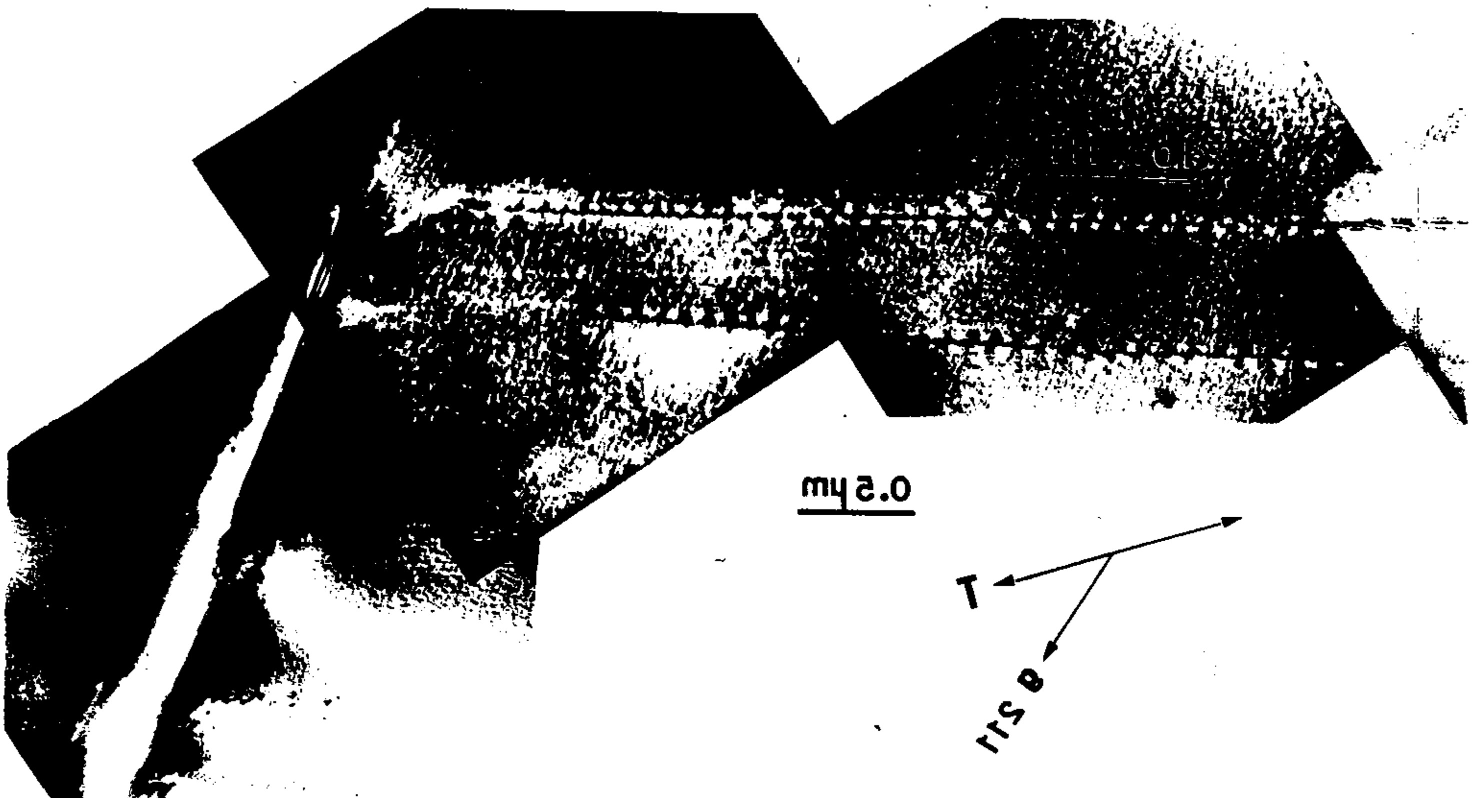
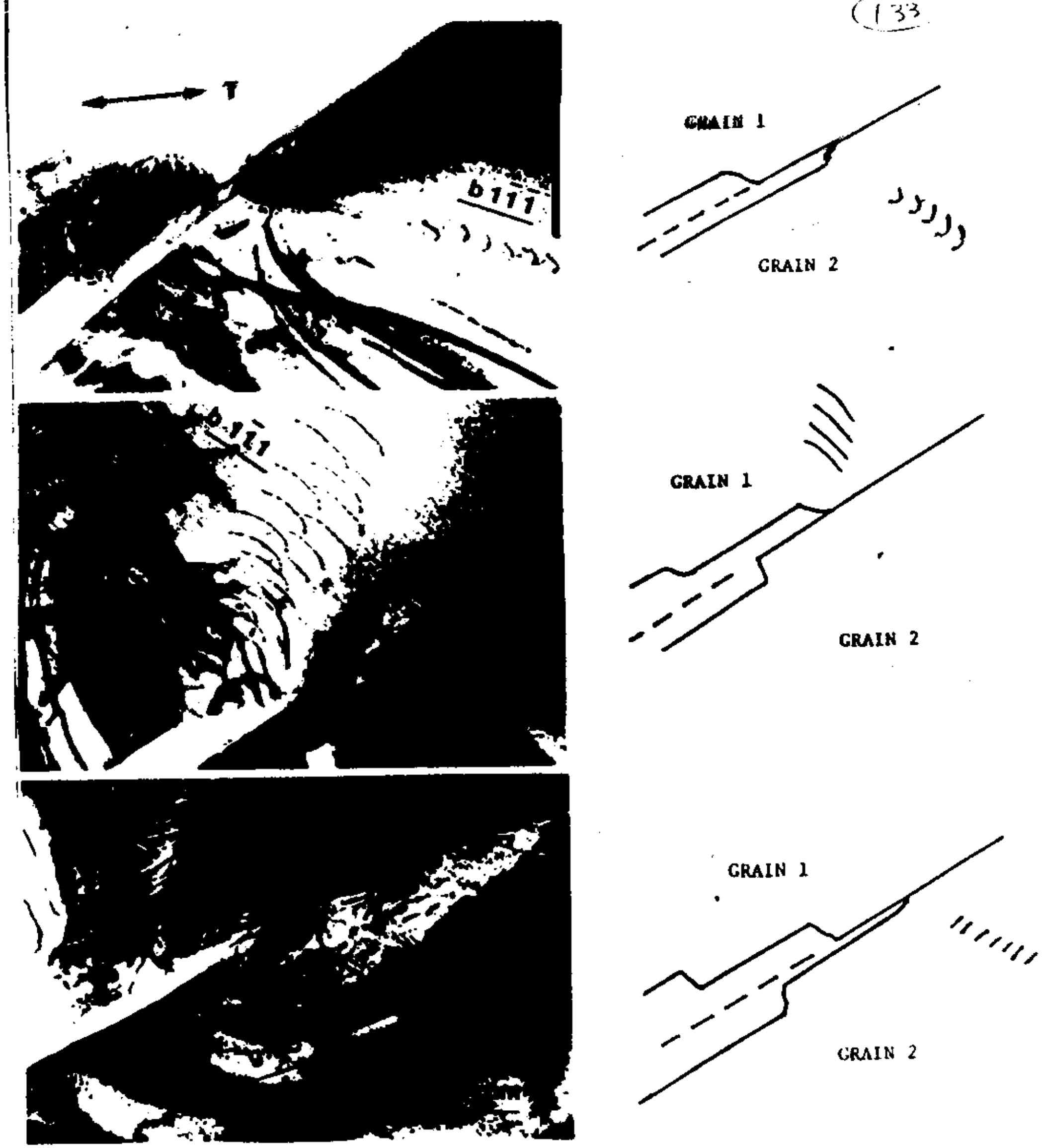


Fig. 5. Mode III Crack along grain boundary near Σ 19. Dislocations are in the form of an inverse pile-up against crack.

Fig. 3. Propagation of an intergranular crack.



θ /[H K L]	SYSTEM	$\Delta\theta$ / $\Delta\theta_{max}$
31.83°/[8 5 4]	Σ 35, 34.04°/[2 1 1]	1.92

Fig. 4. Dislocation emission from an intergranular crack. DFZs are present between crack tip and plastic zones. Alternate of crack propagation and disloction emission is observed.

Fig. 8. Steps remain on the fracture surface. The heights of steps correspond to the total Burgers vectors of dislocations emitted and still remaining in the grain.

BOUNDARY	θ /[H K L]	SYSTEM	$\Delta\theta/\Delta\theta_{max}$
1	32.86°/[8 6 3]	Σ 45, 36.87°/[2 2 1]	3.03
2	47.79°/[8 5 3]	Σ 39, 50.13°/[3 2 1]	1.77
3	16.26°/[9 1 3]	—	—
4	60.15°/[7 6 4]	Σ 17, 61.93°/[2 2 1]	1.88
5	15.10°/[9 4 3]	—	—

Fig. 2. Intergranular crack. Crack prefers to propagate along large angle boundaries.

External Sources

1. Problem is "Plastic Polarizable Mat'l"

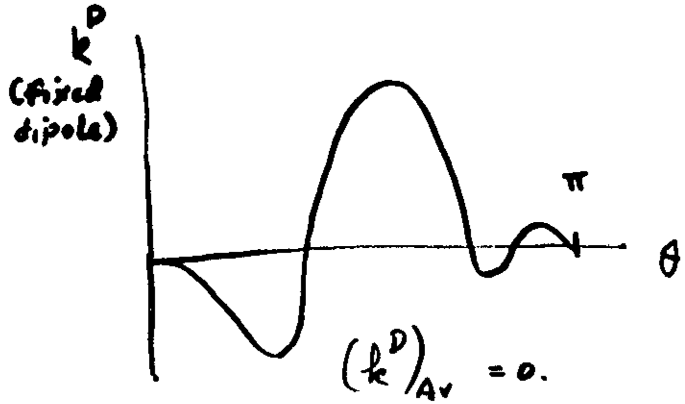
B is conserved

2. Role of anti shielding (?).

$$K = k + k^D$$

$$k^D = \frac{\mu b}{8\pi}\left(\frac{1}{\sqrt{\xi}} + \frac{1}{\sqrt{\xi'}}\right)$$

Anti Shielding always present when $b<0$.



General Results (2D)

1. Stationary Crack

k^D is antishielding

(Narita Experiments)

2. Uniformly moving Crack

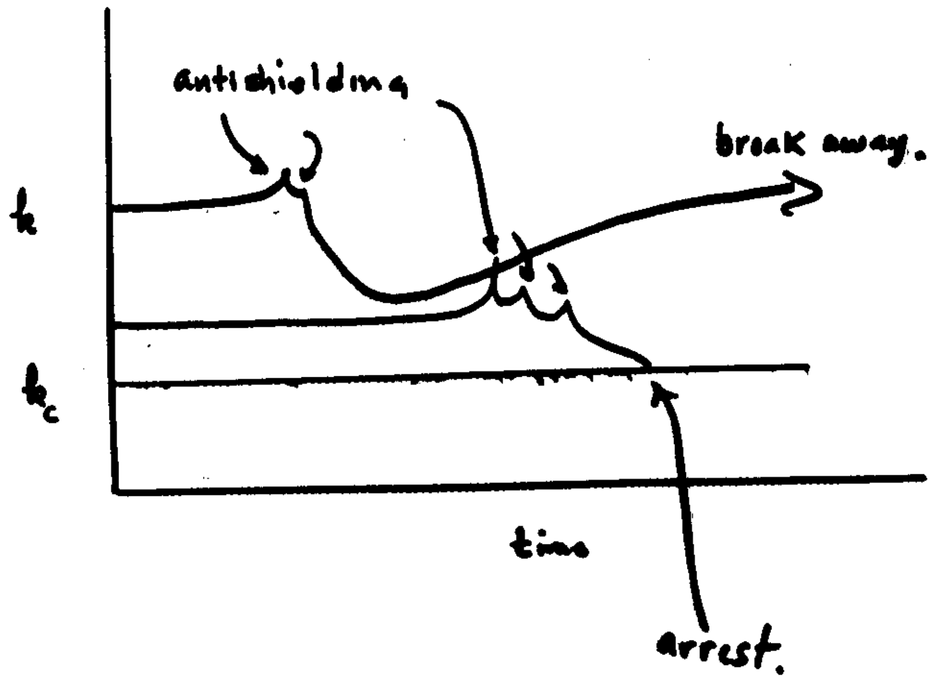
k^D is shielding

3. Time Dependent Motion - Sources are discretely distributed

k^D has both regimes

Zhou self consistent calculation of single source

Other work by Lee, Gerberich, Weertman, Rice, ..



modeling

1. Source. critical stress for (multiple) operation
2. $v(\sigma)$ for dislocations
3. $v(k)$ for crack.

Conclusions

1. Ductility controlled by
   intrinsic processes
   stable (?)
   extrinsic processes
   inherently instable.

2 No complete theory
   Elements for understanding
   challenge for modelers

SUMMARY

- Most Effective Toughness Mechanism is Athermal Disl. Emission
- Dislocation Shielding Leads to Unstable Crack. (? – Can crack be completely shielded)
  Dislocation Free Zone Controversy.
- Criterion for Emission
  - a) Atomic (+ Chemical) force laws at tip.
  - b) Loading Mode
  - c) Thermal emission easy (?)
    but Si studies suggest complicati
- Critical Velocity for Fast Cracking in Ductile Matl.
  - a) Arrest Mechanism :
    Ligaments
    Is Iron special ??

III Dynamic Brittle Cracking of Ductile Metals

Stress Corrosion of Brass, Cu, Au — Pugh / Flanagan / Sieradzki + Newman

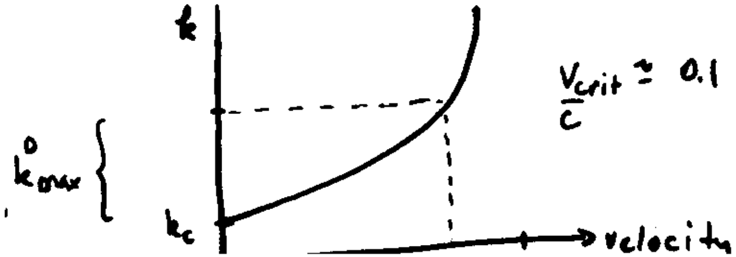
Cu/Bi: Wong.

1. How are cracks generated?
2. Existence proof.?
3. How do they stop?

(2) Paradox

Since a crack has no inertia, any virtual emission will stop crack.

$$k^D \simeq \frac{\mu b}{\sqrt{2\pi r}} \qquad \text{Max}: \quad k^D_{max} = \frac{\mu b}{\sqrt{2\pi r_0}}$$



$$\frac{V_{crit}}{c} \simeq 0.1$$

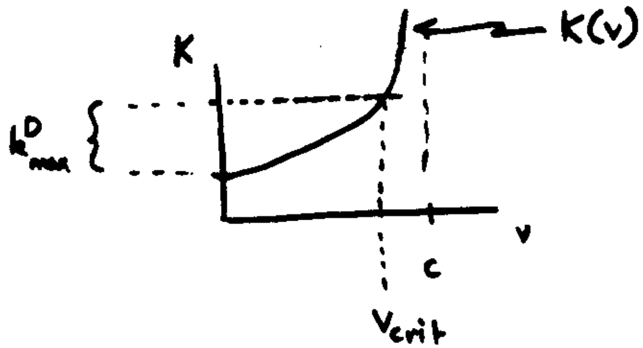
Pugh, See NATO Atomistics of Fracture

Dynamic Cleavage in Ductile Matls.

Is there a critical velocity above which emission stops??

- Crack has no inertia (?) [Sieradski et al. / Lund.

- Max k^D_{shield} exists, If $K > k_g + k^D_{max}$



FRACTURE OF INTERFACES

D. Lashmore
[illegible]
[illegible]

INTRODUCTION

1. Lashmore Multilayers (Electrochemical)
2. Generic Brittle / Ductile
3. Intrinsic / Extrinsic Ductility

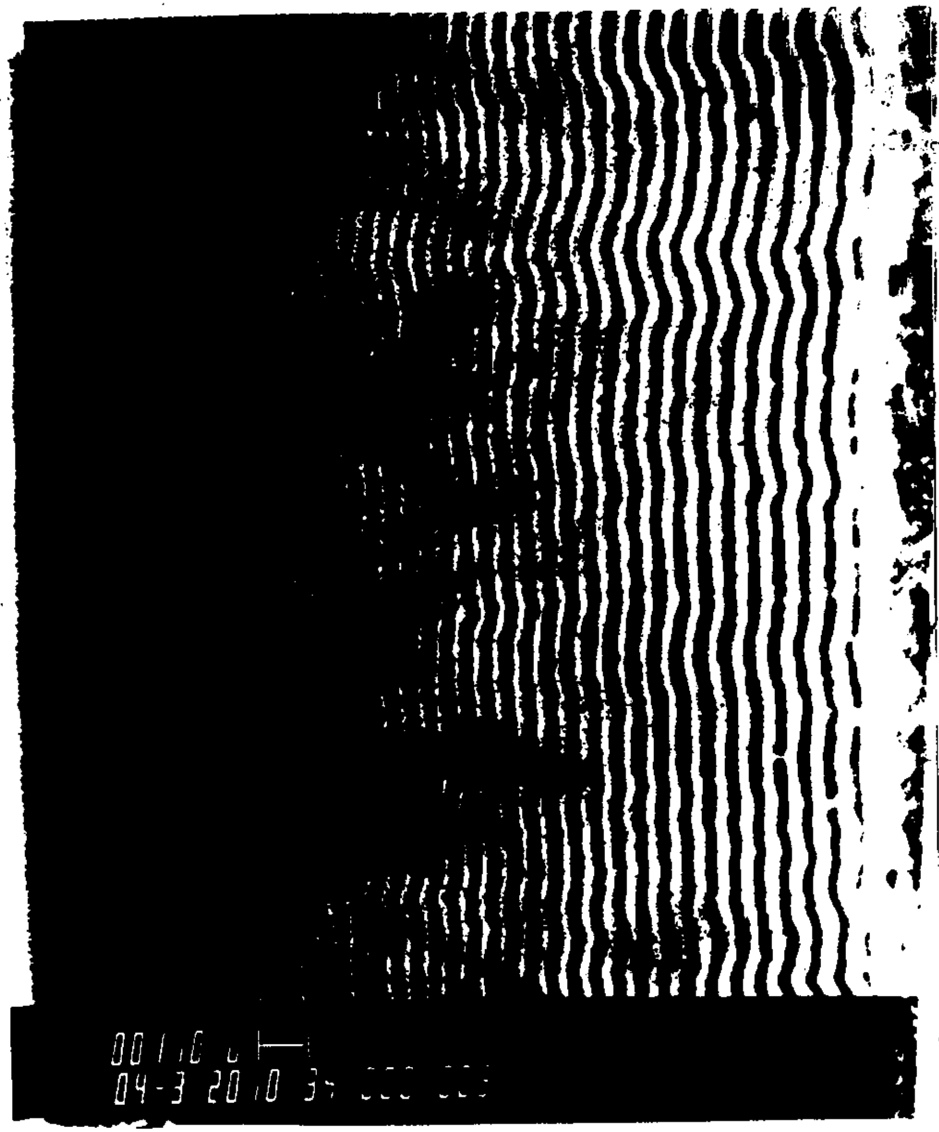
Green's Fns For Lattices

Interfacial Crack.

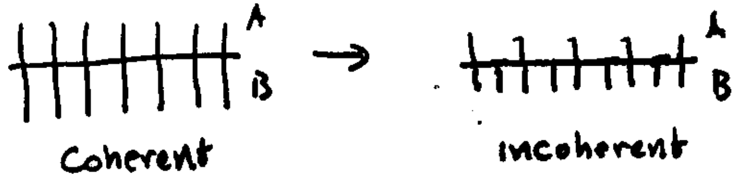
Future Problems.

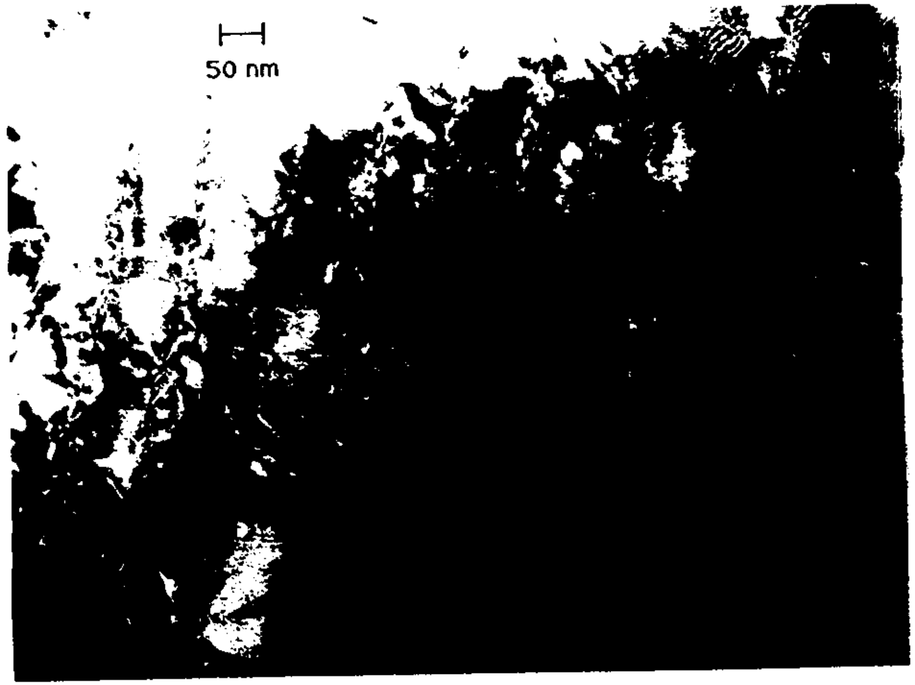
LASHMORE'S MULTILAYERS:

1. Prepared by electrodeposition
2. Large regions of perfection (cm!)
3. Layer thicknesses 100Å →
4. Variety of metals Cu/Ni Cu/Fe/ Cu/Cr..
5. Highly perfect interfaces (extensive Xray satellite structure)

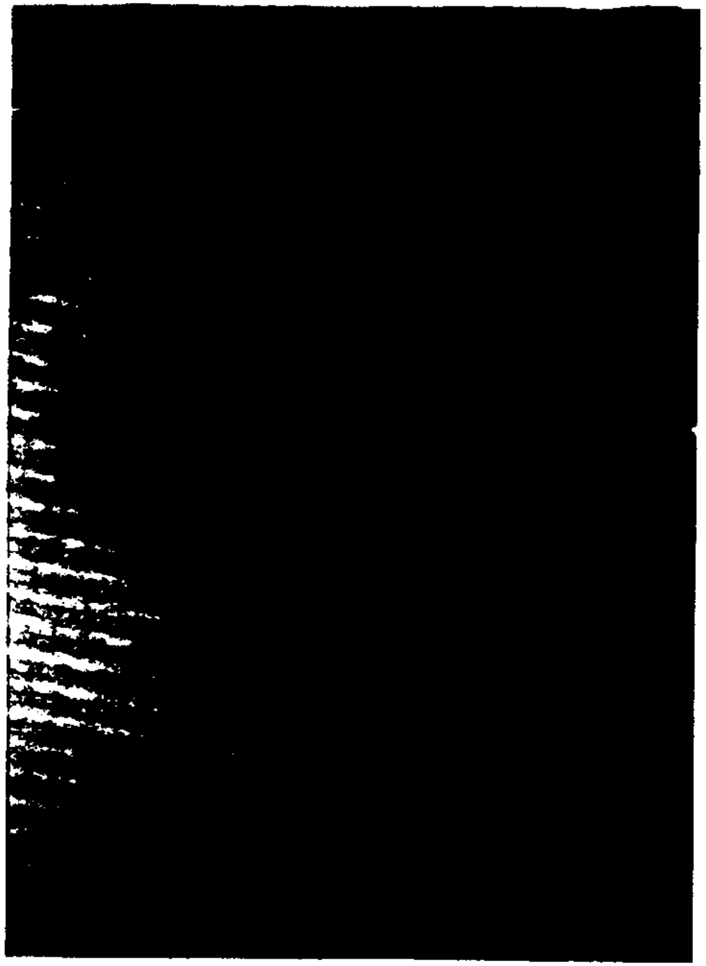


Scanning Electron micrograph of a cross section of a graded alloy with periodicity varied from 30 nm to 300 nm.

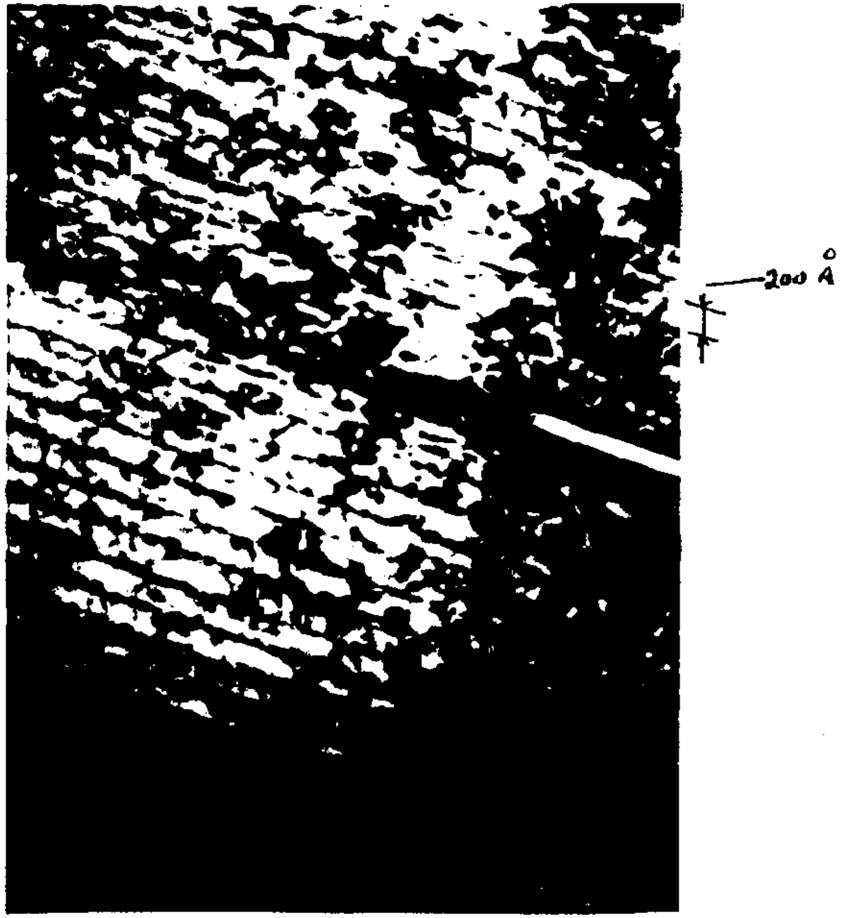




Transmission Electron Micrograph of a cross section of 50 nm Cu/Ni multilayer alloy. Note that at this larger wavelength both boundaries are incoherent at that all dislocations are pinned within the layer.



100 Å Cu/ 100 Å Ni

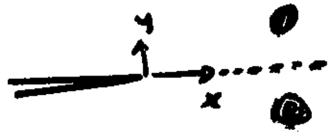


100 Å Cu/ 100 Å Ni
potentiostatic

Interfacial Cracks
Elastic Solns

(149)

England
Trans ASME
June 1965 p400



Goursat Eqns: (Isotropic)

$$\begin{cases} \sigma_{22} - i\sigma_{12} = \varphi' + \bar{\omega}' + (z-\bar{z})\,\bar{\varphi}'' \\ 2\mu u = \kappa\varphi - (z-\bar{z})\,\bar{\varphi}' - \bar{\omega} \end{cases}$$

B.C.
σ_{22}, σ_{12} cont. $x>0$
u cont. $x>0$

Hence:
$$\mu_2\{\kappa_1\varphi_1 - \bar{\omega}_1\} = \mu_1\{\kappa_2\varphi_2 - \bar{\omega}_2\} \quad \text{on } x>0.$$

As before Define $f^*(z) = \overline{f(\bar{z})}$

$$\{\underbrace{\mu_2\kappa_1\varphi_1 + \mu_1\omega_2^*}_{x>0}\}^+ = \{\underbrace{\mu_1\kappa_2\varphi_2 + \mu_2\omega_1^*}_{x>0}\}^- = \xi^{\pm}(z)$$

Likewise
$$\{\varphi_1' - \omega_2^{*\prime}\}^+ = \{\varphi_2' - \omega_1^{*\prime}\}^- = \theta^{\pm}(z)$$

where $\xi(z)$, $\theta(z)$ are entire complex fns.

Boundary Conditions on Crack become:

solve for φ, ω:

$$\varphi_1'^+ = \frac{\xi'^+ + \mu_1\theta'^+}{\mu_2\kappa_1 + \mu_1} \quad ; \quad \omega_2^{*\prime} = \frac{\xi'^+ - \mu_2\kappa_1\theta'^+}{\mu_1 + \mu_2\kappa_1}$$

$$\varphi_2'^- = \frac{\xi'^- + \mu_2\theta'^-}{\mu_2 + \mu_1\kappa_2} \quad ; \quad \omega_1^{*\prime} = \frac{\xi'^- - \mu_1\kappa_2\theta'^-}{\mu_2 + \mu_1\kappa_2}$$

Cont

on Crack $\quad \sigma_{22} - i\sigma_{12}\Big]^{\pm} = -p(x)$

On each surface, expand in terms of ξ, θ:

$$\frac{\mu_1}{\mu_1+\mu_2\kappa_1}\theta^+ - \frac{\mu_1\kappa_2}{\mu_2+\mu_1\kappa_2}\theta^- + \frac{1}{\mu_1+\mu_2\kappa_1}\xi'^+ + \frac{1}{\mu_2+\mu_1\kappa_2}\xi'^- = -\tfrac{1}{2}p$$

$$\frac{-\mu_1}{\mu_1+\mu_2\kappa_1}\theta^+ + \frac{\mu_1\kappa_2}{\mu_2+\mu_1\kappa_2}\theta^- + \frac{1}{\mu_1+\mu_2\kappa_1}\xi'^+ + \frac{1}{\mu_2+\mu_1\kappa_2}\xi'^- = -\tfrac{1}{2}p$$

Subtract: $\theta^+ - \theta^- = 0 \implies$ **θ is continuous**

Add:

$$\boxed{\begin{gathered} \xi^+ + \alpha\,\xi^- = -\frac{\mu_1+\mu_2\kappa_1}{2}\,p(x) \\ \alpha = \frac{\mu_1+\mu_2\kappa_1}{\mu_2+\mu_1\kappa_2} \end{gathered}}$$

Hilbert Problem

Cont

Consider Unloaded Crack

$\xi^+ = -\alpha\, \xi^-$

Consider

$f(z)$

$$f(z) = e^{\gamma \ln z} = e^{\gamma(\ln|z| + i\theta)} = e^{(\frac{1}{2}+ib)(\cdots)}$$

$$= \frac{e^{i\theta/2}}{\sqrt{r}}\; e^{ib \ln|z|}\; e^{-b\theta}$$

$$\frac{f^+}{f^-} = e^{i\pi} e^{-2\pi b} = -e^{-2\pi b}$$

$$= -\ln\frac{1}{2\pi b}$$

Thus $\alpha = \ln \frac{1}{2\pi b}$

A fundamental soln becomes

$$\xi = \frac{e^{i\theta/2}}{\sqrt{r}} \left[e^{-b(\theta - i \ln r)} \right]$$

$2\pi b = e^{-\alpha}$

This gives oscillatory displacements!

Cont

1. Characteristics of elastic Soln:

- oscillatory closing at crack tip.
  Cannot be physical — if ~~closure~~ then repulsive forces ~~generated~~.
  Or dislocation (?)
- Occurs near tip — crack must be long.

$$l_c = \frac{\text{closure region}}{\text{crack length}} \sim 10^{-4}$$

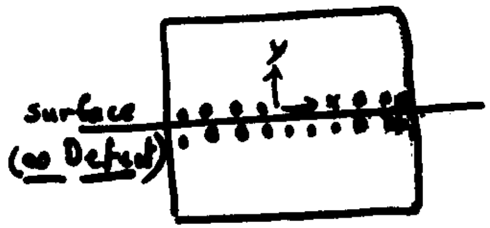
(atomic ??)

Atomic Description

G for Surface

(153)

Surface is:
∞ in extent
homogeneous in x



Have terms like

$$G\delta\phi G^{\#}$$
$$= \sum G(l_x - l_x'') \, \delta\phi(l_x'' - l_x''') \, G^{\#}(l_x''' - l_x') \, \delta|$$
$$= \underbrace{\sum G(q)\delta\phi(q)\, G^{\#}(q)}_{\text{single term from } q.} \, e^{iq(l_x - l_x')} \quad \underbrace{\delta\phi(}_{\text{finite}}$$

from F. Xform.

Solve a finite set of eqns.
(Finite matrices)

For Interface

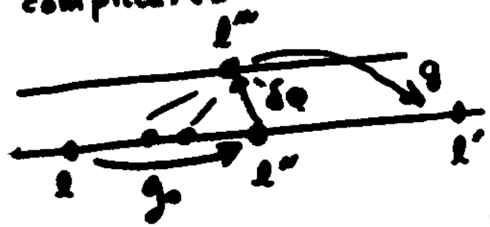
ϕ, G periodic in x, y. Not z

In 2D Dyson eqn is

$$G(q; l_y, l_y') + G^0(q; l_y, l_y'')\,\delta\varphi(l_y'', l_y''')\, G(q; l_y''', l_y') = G^0(q, l_y, l_y')$$

$$G(l_x - l_x'; l_y, l_y') = \sum G(q; l_y, l_y')\, e^{-iq(l_x - l_x')}$$

$G^0\delta\phi G$ is complicated matrix product. (Analogy to Feynman Dia



$$\delta\varphi_{ij} = \begin{pmatrix} \alpha & \beta \\ \beta & \gamma \end{pmatrix}$$

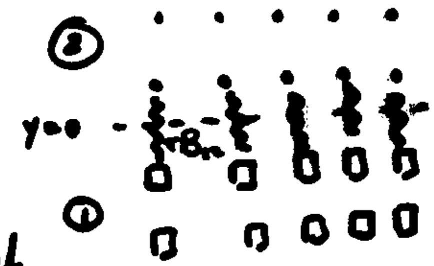
For Interfacial Crack
$G^0 \to G^s \to G^i \to G^{crack}$

Interface G

Two dual xtals

$A_1, B_1, C_1 \cdots$

$A_2\ B_2\ C_2 \cdots$



create surface in each

) Glue together at y=0. B_{12}

$$\delta\Phi_{y} = \begin{array}{c|cc} & ① & ② \\ \hline ① & -B_{12} & B \\ ② & B_{12} & -B \end{array}$$

) $\delta\Phi$ again homogeneous in x :

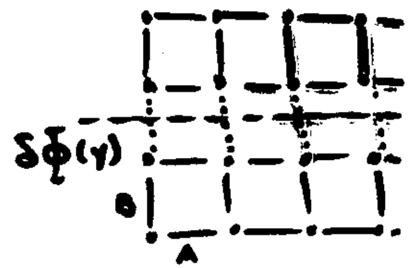
$$G^{(11)}_{inter} = \frac{G^{①}_{surf}\left(1 + B_{12}\, G^{②}_{surf}\right)}{\Delta}$$

$$G^{(12)}_{inter} = \frac{B_{12}\, G^{(2)}_{surf} G^{(1)}_{surf}}{\Delta}$$

$$G(22)_{inter} = \frac{G^{(2)}_{surf}\left(1 + B_{12}\, G^{(1)}_{surf}\right)}{\Delta}$$

A specific Example

$$\delta\Phi(y) = \begin{array}{c|cc} & -1/2 & 1/2 \\ \hline -1/2 & B & -B \\ 1/2 & -B & B \end{array}$$

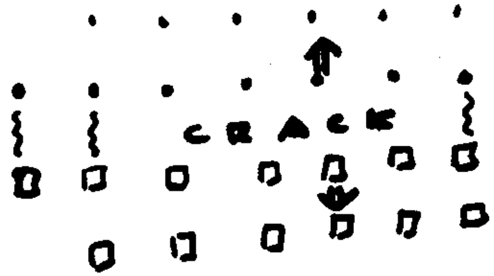


$$G_{surf}\left(l_x - l_x' ; -1/2 ; -1/2\right) = g^{(0)}_{(0,0)} + g^{(1)}_{(0,1)}$$

$$G_{surf}\left(l_x - l_x' ; -1/2 , +1/2\right) = 0$$

CRACK

Annihilate bonds at interface to make crack

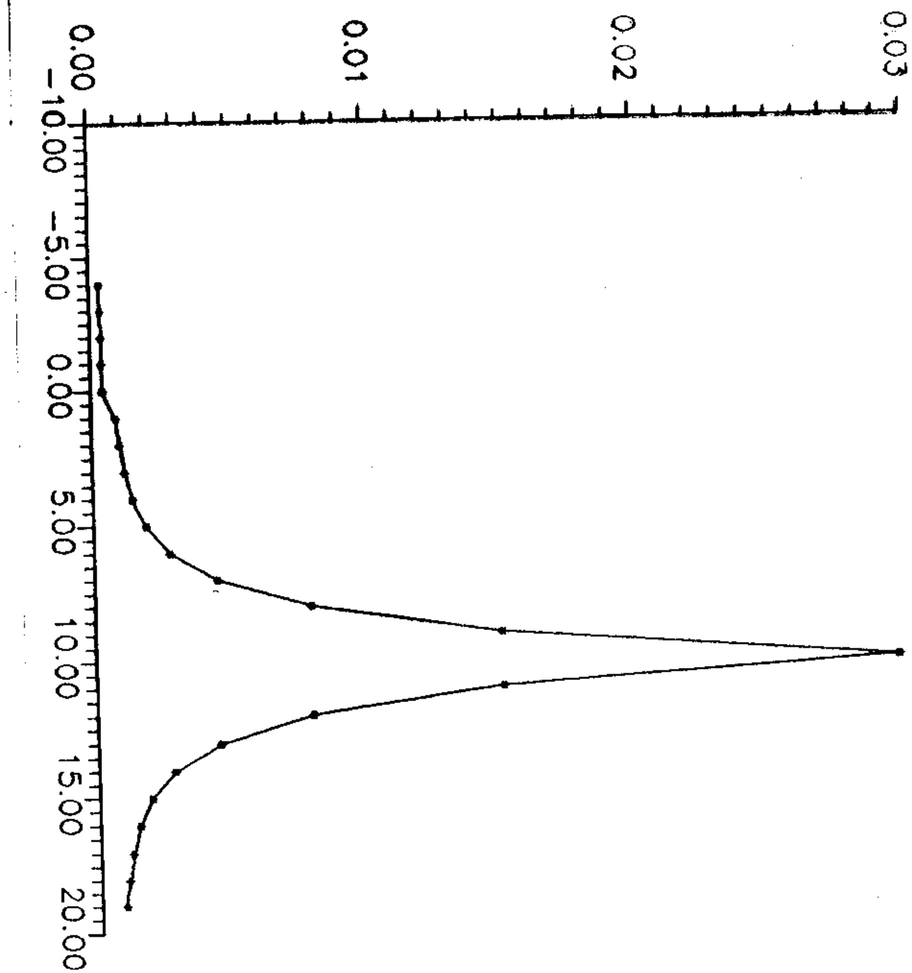


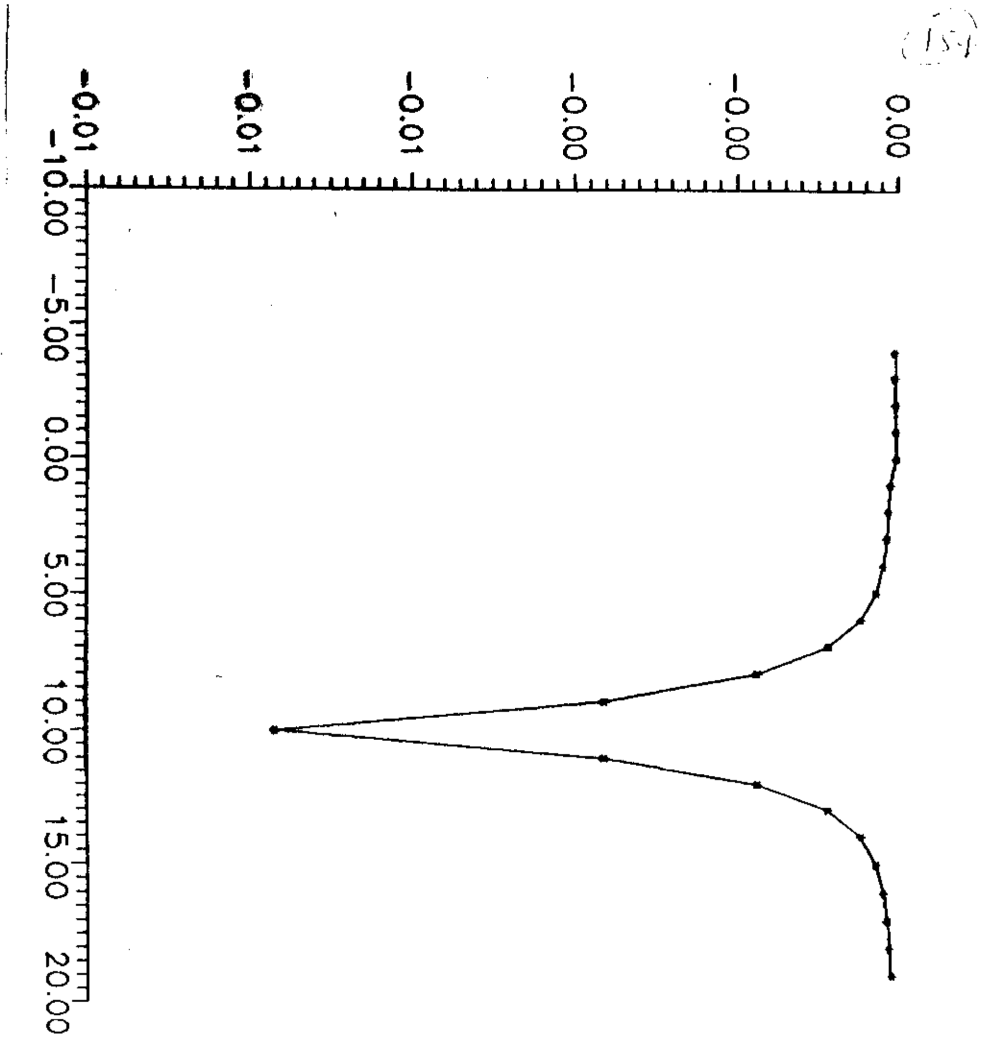
$$\delta\Phi_{crack} = \begin{bmatrix} +B_{12} & -B_{12} \\ -B_{12} & +B_{12} \end{bmatrix}$$

For cleavage surface (finite

Now solve finite matrix eqns. for crack displ.

$$G^*_{crack} = G_{inter} + \sum_{crack} G_{inter}\, \delta\phi_{crack}\, G^*_{crack}$$



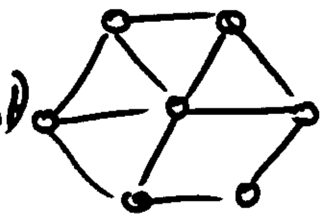


Interfacial Crack in 2D Hex Lattice

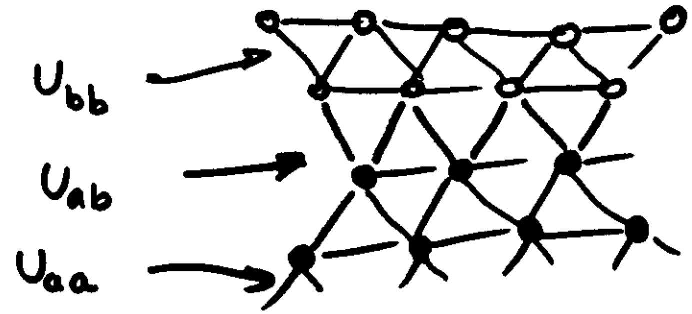
Bonds are nn.

$U = U(|\underline{r}|)$

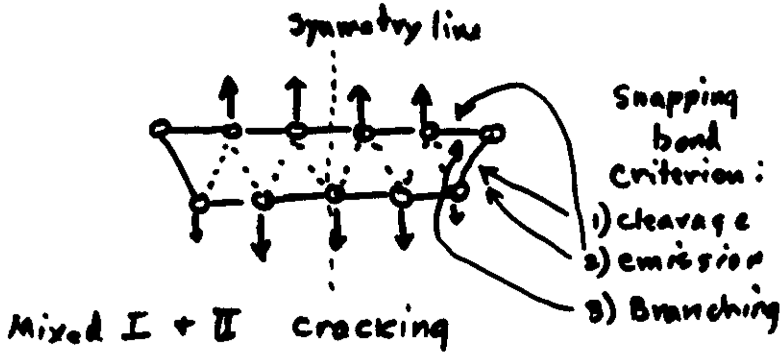
(no bending component)



Interface

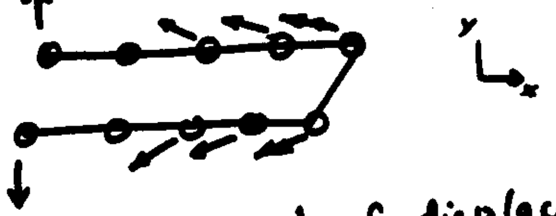


Crack



A Result of work on Interfacial Cracks

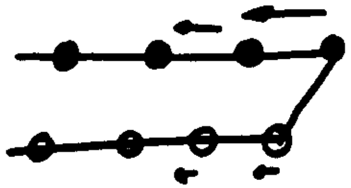
Single Xtal



Note large "Poisson ratio Effect".

x component of displacement balanced at tip.

Interface



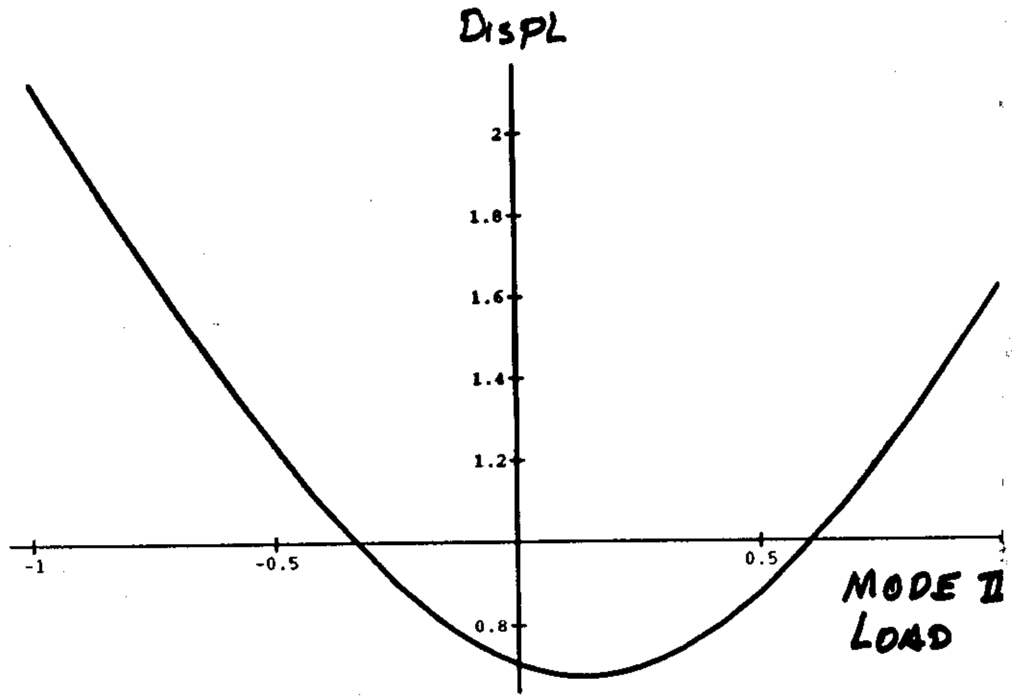
Large inhomogeneous strain at tip.

Thus Cleavage more difficult!

Detailed study shows that all processes at tip (cleavage, emission, branching) are altered by interface in rather complicated way. Some effects driven by lattice geometry; others by bond changes.

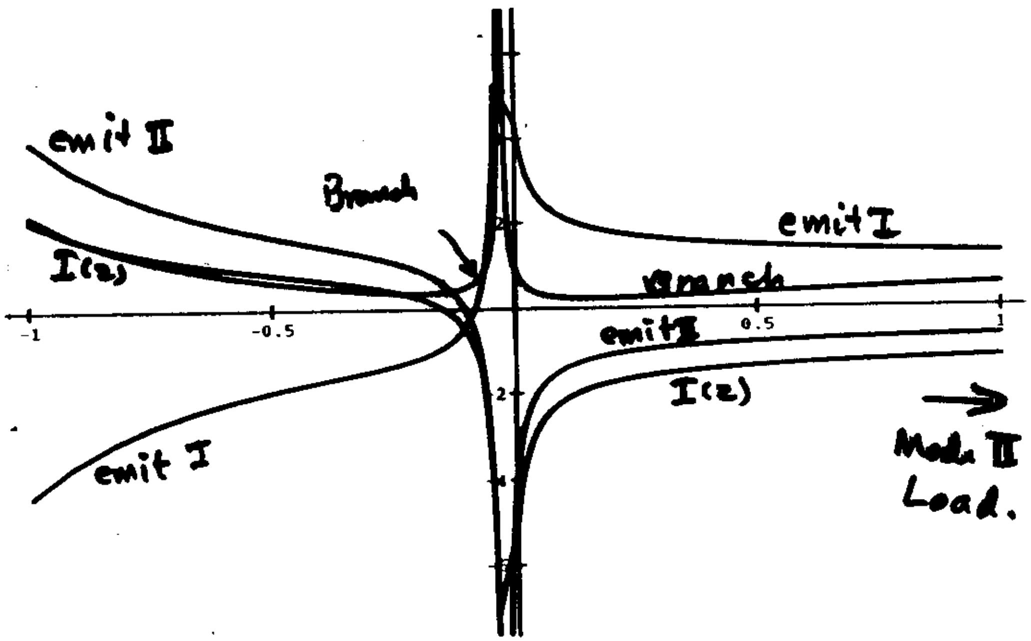
CLEAVAGE DISPLACEMENT

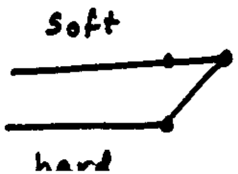
HEX XTAL

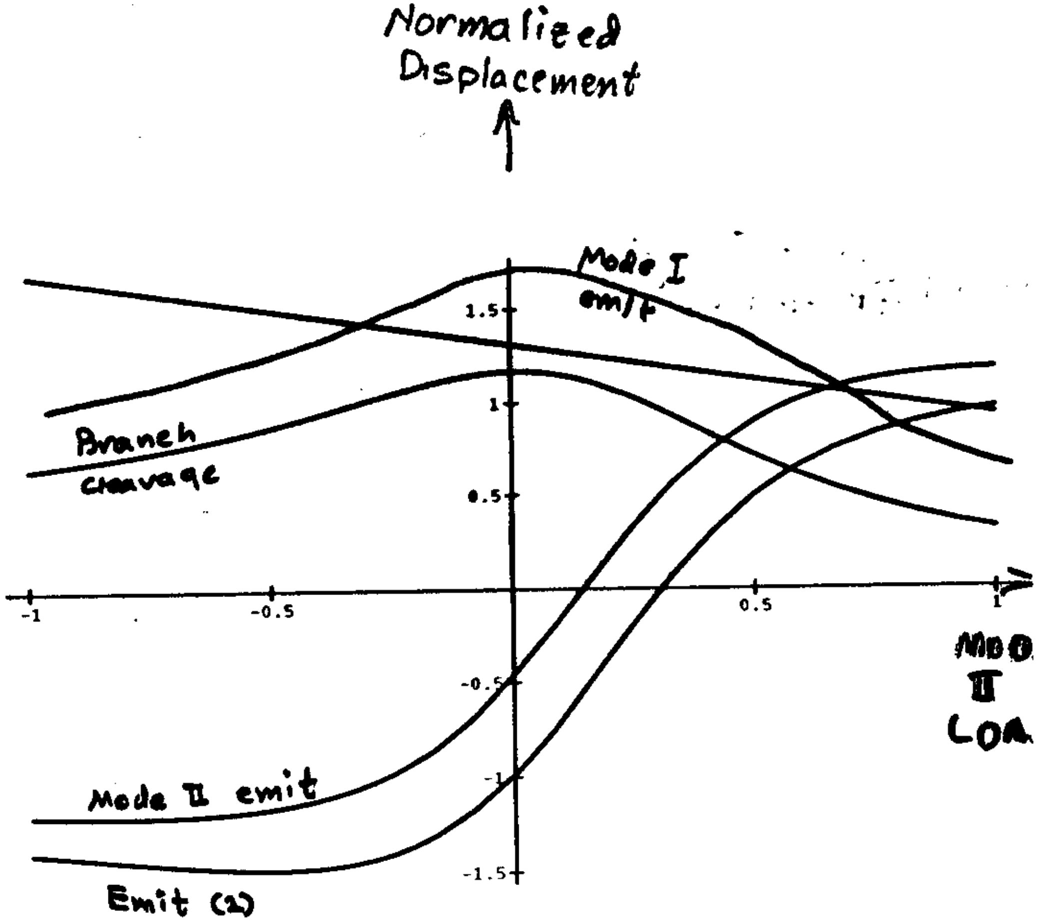


NO INTERFACE

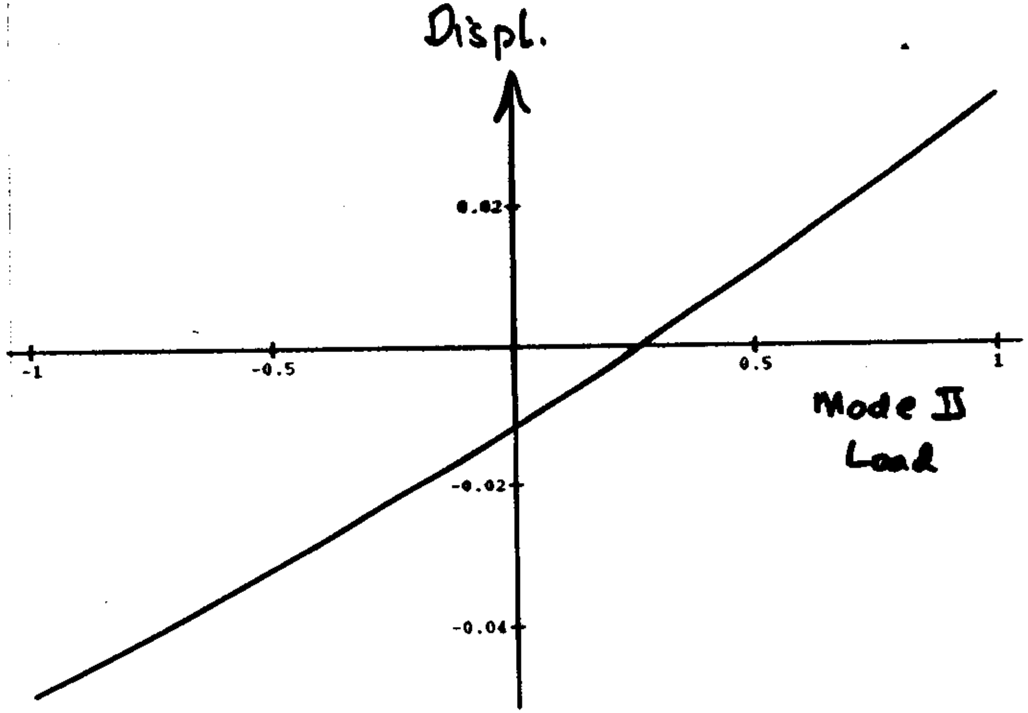
Displacements

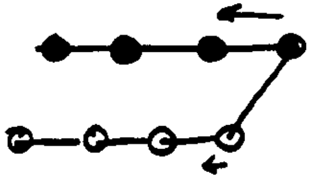






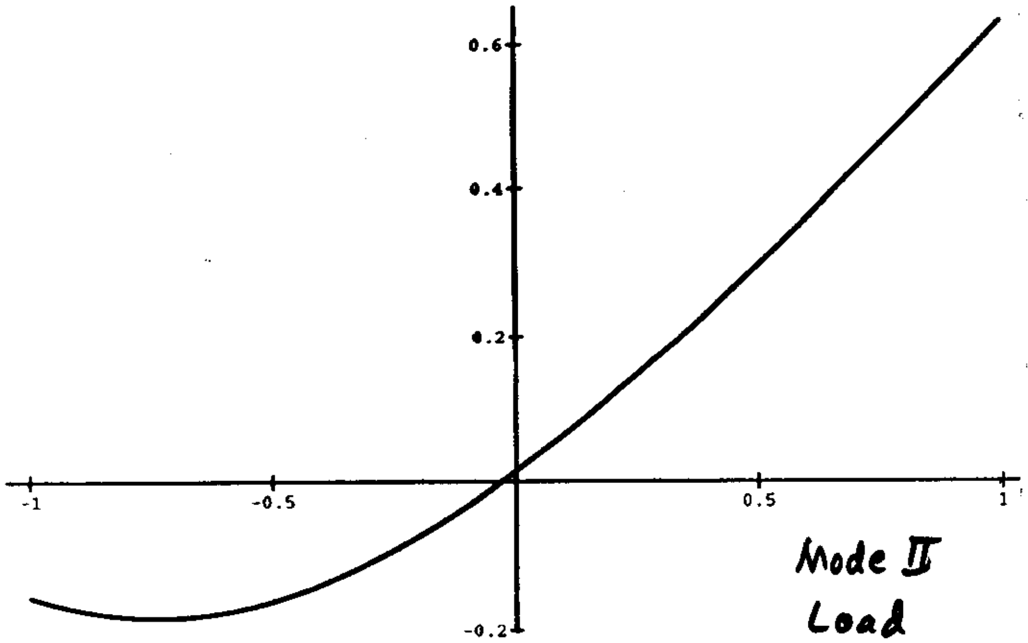
INTERFACIAL CLEAVAGE DispL



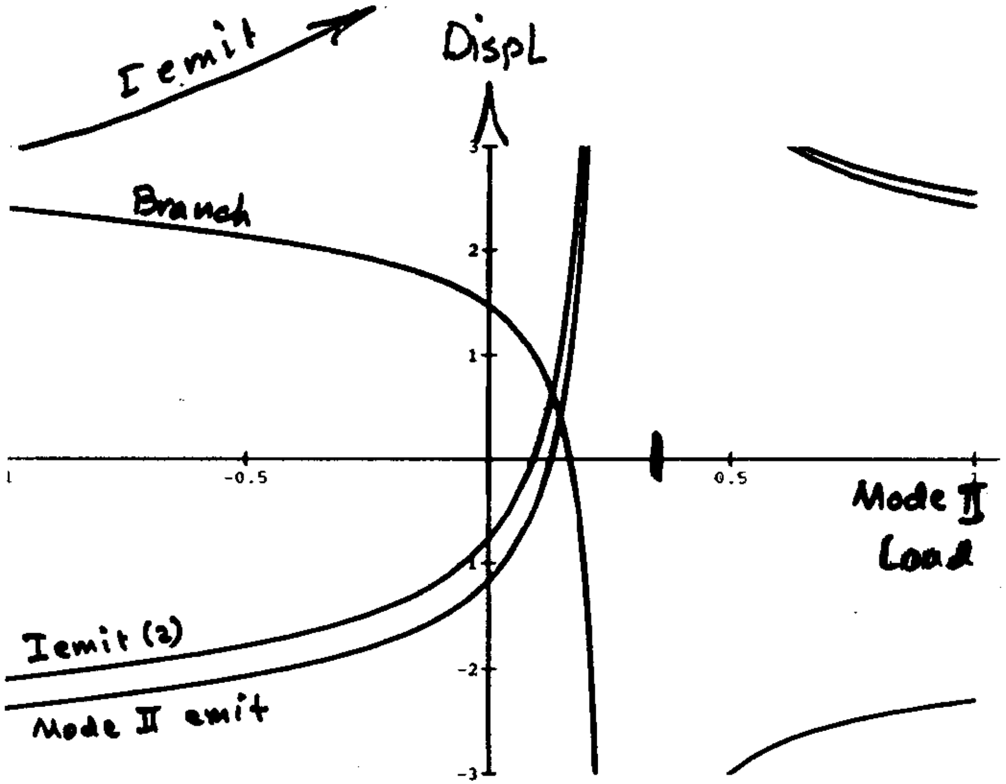


Cleavage inhibited!

CLEAVAGE DispL



INTERFACIAL Displacement



Conclusions

INCREASING THEORETICAL CHALLENGE

1. Methods to model realistic atomic processes at crack tips (including interfaces) are coming to hand.
   - intrinsic ductility
   - chemical Effects.

2. Some insights into "several" body Shielding available.
   (3D/2D transition Big Problem)

3. Translation to Continuum average properties Not Available
   - Asymptotic Relations
   - Many body Crack - dislocation inter.

   NEW IDEAS NEEDED

4. Can now predict that theory + Modelin of materials will generate a revolution in [illegible] MS is done in future!