INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE CENTRATOM TRIESTE

SMR.550 - 13

SPRING COLLEGE IN MATERIALS SCIENCE ON

"NUCLEATION, GROWTH AND SEGREGATION IN MATERIALS SCIENCE AND ENGINEERING"

(6 May - 7 June 1991)

"EXTENDED DEFECTS"

E.J. SAVINO
Proyecto Multinacional de Investigacion y
Desarrollo en Materiales - OEA-CNEA
Av. del Libertador 8250
1429 Buenos Aires
Argentina

SPRING COLLEGE IN MATERIALS SCIENCE ON
"NUCLEATION, GROWTH AND SEGREGATION IN MATERIALS SCIENCE AND ENGINEERING" - I.C.T.P., 6 MAY-7 JUNE, 1991

"EXTENDED DEFECTS", E.J. SAVINO - LECTURE NOTES

INDEX

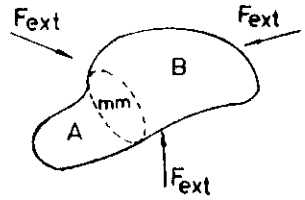
1. BRIEF INTRODUCTION TO ELASTICITY

1.1. ELASTIC MEDIUM

In an elastic medium the displacements are uniquely determined by the applied forces. The strain response to each applied stress (or viceversa) has a unique equilibrium value and the response is achieved instantaneously. As a corollary, a complete recoverability of the response is also instantaneous uppon release of the applied stress/strain. When the response is linear we are within the limit of linear elasticity and Hooke's law applies.

1.2. STRESS

Suppose a body in equilibrium under a set of applied forces.

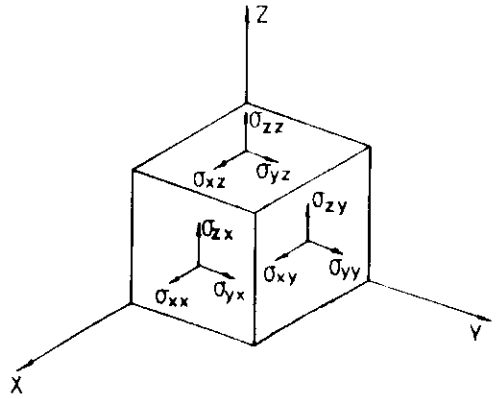


The domain B of the body experiences the forces applied on A through the surface mm.

⇓

There is an internal force $\delta\underline{F}$ on every surface element $\delta\underline{A}$ of mm such that: $\delta\underline{F} / \delta A \neq 0$.

In the limit $\delta\underline{A} \to 0$, the stress $\sigma_{ij} = \delta F_i / \delta A_j$.



Equilibrium ⇒

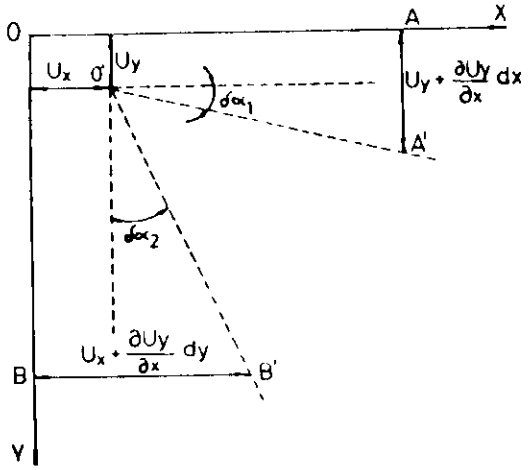
$\sigma_{ij} = \sigma_{ji}$ and $\delta\sigma_{ij} / \delta_{xj} + f_i = 0$

No torque

f_i: i^{th} component of the body force per unit volume.

1.3. STRAIN

Displacement field: $\underline{u} = \underline{u}(x, y, z)$



A Q + dx x̂ B Q + dy ŷ

$$u_x(A) - u_x(Q) = \frac{\partial u_x}{\partial x} dx = \epsilon_{xx} dx \quad \rightarrow \quad \frac{\Delta l_x}{l_x} = \epsilon_{xx}$$

$$tg\ \delta\alpha_1 = \frac{u_y + \frac{\partial u_y}{\partial x} dx - u_y}{dx} = \frac{\partial u_y}{\partial x}$$

$$tg\ \delta\alpha_2 = \frac{\partial u_x}{\partial u_y}$$

Angle distortion:

$$\gamma_{xy} = \frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}$$

Strain:

$$dx'_i = dx_i + \frac{\partial u_i}{\partial x_j} dx_j = dx_i + \nabla_j u_i\, dx_j = dx_i + (\epsilon_{ij} + \omega_{ij})\, dx_j$$

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

Strain $\neq 0$ if $i \neq j$
rigid rotation

Volume change: If $V = dxdydz$

$$\Delta V = V' - V = \Pi_i (1 + \epsilon_{ii})\, dx_i - \Pi_i\, dx_i = \mathrm{Tr}\ \underline{\epsilon} \cdot V$$

1.4. ENERGY

Energy density: $d\omega = \Sigma_{\alpha\beta}\, \sigma_{\alpha\beta}\, d\epsilon_{\alpha\beta}$

Just as the equilibrium imposes restrictions on $\underline{\sigma}$, compatibility imposes restrictions on $\underline{\epsilon}$.

For example, planar strain $\epsilon_z = 0$ in cylindric coordinates

$$\underline{u} = u_r(r)\hat{r} \rightarrow \epsilon_r = \partial u / \partial r\ ,\ \epsilon_\theta = u / r$$

$$\rightarrow \epsilon_r = \partial(r\epsilon_\theta) / \partial r$$

1.5. STRAIN AND COMPATIBILITY IN CARTESIAN COORDINATES

In general, as the strain tensor ϵ_{ij} has six components and depends on the six components for the displacement vector $\underline{u}$, the tensor components have to fulfil a set of relations among themselves. These are deduced from the relation:

$$\epsilon_{ij} = 1/2\ (\partial u_i/\partial x_j + \partial u_j/\partial x_i)$$

The compatibility condition is, in Cartesian coordinates:

$$\epsilon_{pki}\ \epsilon_{qlj}\ \epsilon_{ij,kl} = 0$$

where ϵ_{pki} is the permutation tensor:

ϵ_{pki} = 1 for the even permutation of 1, 2, 3

-1 for the odd permutation of 1, 2, 3

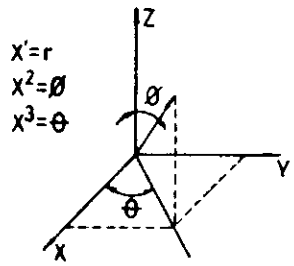
0 for other cases

and

$$\epsilon_{ij,kl} = \frac{\partial}{\partial x_k}\ \frac{\partial}{\partial x_l}\ \epsilon_{ij}$$

1.6. COMPATIBILITY IN SPHERICAL COORDINATES

The relation between strain and displacement field deduced above is a particular form of the so-called kinematic relations, in spherical coordinates these are:



$$\epsilon_{11} = \frac{\partial u_1}{\partial x^1}$$

$$\epsilon_{22} = \frac{\partial u_2}{x^1\,\partial x^2} + \frac{u_1}{x^1}$$

$$\epsilon_{33} = \frac{1}{x^1\ sen\ x^2}\ \frac{\partial u_3}{\partial x^3} + \frac{1}{x^1}\ u_1 + \frac{cotg\ x^2}{x^1}\ u_2$$

$$\epsilon_{12} = \frac{1}{2}\left(\frac{1}{x^1}\ \frac{\partial u_1}{\partial x^2} + \frac{\partial u_2}{\partial x^1} - \frac{u_2}{x^1}\right)$$

$$\epsilon_{23} = \frac{1}{2}\left(\frac{1}{x^1\ sen\ x^2}\ \frac{\partial u_2}{\partial x^3} + \frac{1}{x^1}\ \frac{\partial u_3}{\partial x^2} - \frac{cotg\ x^2}{2\ x^1}\ u_3\right)$$

$$\epsilon_{13} = \frac{1}{2}\left(\frac{1}{x^1\ sen\ x^2}\ \frac{\partial u_1}{\partial x^3} + \frac{\partial u_3}{\partial x^1} - \frac{u_3}{x^1}\right)$$

While the equilibrium equations are:

$$F_1 = \frac{1}{(x^1)^3}\frac{\partial}{\partial x^1}\left((x^1)^2\,\sigma_{11}\right) + \frac{1}{x^1\,sen\,x^2}\frac{\partial}{\partial x^2}\left(sen\,x^2\,\sigma_{12}\right) + \frac{1}{x^1\,sen\,x^2}\frac{\partial}{\partial x^3}\left(\sigma_{13}\right) - \frac{1}{x^1}\left(\sigma_{22}+\sigma_{33}\right)$$

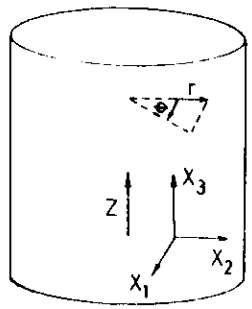
$$F_2 = \frac{1}{(x^1)^3}\frac{\partial}{\partial x^1}\left[(x^1)^3\,\sigma_{12}\right] + \frac{1}{x^1\,sen\,x^2}\frac{\partial}{\partial x^2}\left(sen\,x^2\,\sigma_{22}\right) + \frac{1}{x^1\,sen\,x^2}\frac{\partial}{\partial x^3}\left(\sigma_{23}\right) - \frac{cotg\,x^2}{x^1}\,\sigma_{33}$$

$$F_3 = \frac{1}{(x^1)^3}\frac{\partial}{\partial x^1}\left((x^1)^2\,\sigma_{13}\right) + \frac{1}{x^1\,sen^2\,x^2}\frac{\partial}{\partial x^2}\left(sen^2\,x^2\,\sigma_{23}\right) + \frac{1}{x^1\,sen\,x^2}\frac{\partial}{\partial x^3}\left(\sigma_{33}\right)$$

1.7 COMPATIBILITY IN CYLINDRICAL COORDINATES

Sometimes the compatibility condition is self evident from the geometry of the problem. For example:

Plane strain ($\epsilon_z = 0$) and cylindrical symmetry case:



$x_1 = \theta$

$x_2 = r$

$x_3 = z$

If: $\underline{u} = u_r\,(r, z)$

that is

$u_\theta = 0$

$\partial \underline{u}/\partial\theta = \partial \underline{u}/\partial z = 0$

It results $\epsilon_r = \partial u/\partial r$ (a) , $\epsilon_\theta = u/r$ (b)

By replacing (b) in (a):

$$\epsilon_r = \frac{\partial}{\partial r}\left(r\,\epsilon_\theta\right)$$

compatibility condition

1.8. CONSTITUTIVE EQUATIONS

One needs to relate $\underline{\sigma}$ with $\underline{\underline{\epsilon}}$: constitutive equations.

$$\underline{\underline{\epsilon}} = \underline{\underline{f}} \ (\underline{\sigma}, \ T, \ \text{etc.})$$

Linear elasticity: Hooke's law

$$\sigma_{\alpha\beta} = \Sigma_{\gamma\delta} \ C_{\alpha\beta\gamma\delta} \ \epsilon_{\gamma\delta}$$

$\underline{\underline{C}}$: elastic tensor of rank 4.

Energy density:

$$d\omega = \Sigma_{\alpha\beta} \ \sigma_{\alpha\beta} \ d \ \epsilon_{\alpha\beta} = \Sigma_{\alpha\beta\gamma\delta} \ C_{\alpha\beta\gamma\delta} \ \epsilon_{\gamma\delta} \ d \ \epsilon_{\alpha\beta}$$

We shall later relate these expressions to changes in lattice energy due to homogeneous distortion. For the time being, we keep to the continuum medium approach.

The change in energy due to a distortion of an otherwise stress/strain free medium within the linear elastic approach results:

$$\Phi \ (\underline{\underline{\epsilon}}) = \Phi \ (\underline{\sigma})$$

$$\Phi \ (\underline{\underline{\epsilon}}) = \Phi_o + \int_{\underline{\underline{\epsilon}}=0}^{\underline{\underline{\epsilon}}} d\omega = \Phi_o + 1/2 \ C_{\alpha\beta\gamma\delta} \ \epsilon_{\alpha\beta} \ \epsilon_{\gamma\delta}$$

$$\Phi \ (\underline{\sigma}) = \Phi_o + \int_{\underline{\sigma}=0}^{\underline{\sigma}} d\omega = \Phi_o + 1/2 \ S_{\alpha\beta\gamma\delta} \ \sigma_{\alpha\beta} \ \sigma_{\gamma\delta}$$

where

$$\Phi_o = \Phi \ (\underline{\underline{\epsilon}}=0) = \Phi \ (\underline{\sigma}=0)$$

$\underline{\underline{S}}$: tensor of compliances $\qquad \underline{\underline{S}} = (\underline{\underline{C}})^{-1}$

This implies:

$$C_{\alpha\beta\gamma\delta} = \partial^2 \Phi \ / \ \partial\epsilon_{\alpha\beta} \ \partial\epsilon_{\gamma\delta}$$

$$S_{\alpha\beta\gamma\delta} = \partial^2 \Phi \ / \ \partial\sigma_{\alpha\beta} \ \partial\sigma_{\gamma\delta}$$

1.9 ELASTIC CONSTANTS

As $\sigma_{ij} = \sigma_{ji}$, $\epsilon_{ij} = \epsilon_{ji}$ and $\sigma_{ij} = c_{ijkl}\,\epsilon_{kl} \Rightarrow$

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{jilk}$$

In turn:

$$c_{ijkl} = \partial^2 \Phi / \partial \epsilon_{ij}\,\partial \epsilon_{kl} = c_{klij}$$

It is easy to see c_{ijkl} has:

3	+	(3 x 3)	x 2	= 21
Diagonal		Off diagonal		Independent terms

Voigt notation $c_{mn} = c_{ijkl}$

ij or kl	11	2	33	23	31	12	32	13	21
m or n	1	2	3	4	5	6	7	8	9

$\Rightarrow$ $c_{11} = c_{1111}$, $c_{12} = c_{1122}$, ... etc.

Therefore $\sigma_{ij} = c_{ijkl}\,\epsilon_{kl}$ can be written as:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \\ \sigma_{32} \\ \sigma_{13} \\ \sigma_{21} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{23} \\ \epsilon_{31} \\ \epsilon_{12} \\ \epsilon_{32} \\ \epsilon_{13} \\ \epsilon_{21} \end{bmatrix}$$

Because of symmetry it reduces to:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix}$$

Note that in the reduced scheme the $\gamma_{ij} = 2\,\epsilon_{ij}$ are used.

However, one must remember that for transformation of coordinates $\underline{\underline{c}}$ is a tensor of rank 4. That is if, for coordinates

$x'_i = T_{ij}\, x_j$ where $T_{ij}\, T_{jl} = \delta_{il}$

$\underline{\delta}$: Kronecker delta

It implies:

$$\epsilon'_{ij} = T_{il}\, T_{jm}\, \epsilon_{lm}$$

$$\sigma'_{ij} = T_{il}\, T_{jm}\, \sigma_{lm}$$

and

$$c'_{ijkl} = T_{ig}\, T_{jh}\, c_{ghmn}\, T_{km}\, T_{ln}$$

CAUTION:

Voigt indexes do not correspond to tensor index and c_{mn} is not the mn component of a tensor of rank 2.

1.10. HOOKE'S LAW UNDER DIFFERENT CONDITIONS

Number of independent constants depend of the tension state.

Isotropic solid:

1D: Uniaxial tension, linear answer (extension).

$\sigma = E\epsilon$ 1 constant!

2D , 3D $\Rightarrow$ 2 constants: E, υ ; K, G ; λ, μ

c_{11}, c_{12}

Planar tensions:

$\sigma_3 = \tau_{13} = \tau_{23} = 0$

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{12} & Q_{22} & 0 \\ 0 & 0 & Q_{66} \end{bmatrix} \cdot \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ 2\epsilon_6 \end{bmatrix}$$

$Q_{11} = c_{11}$

$Q_{12} = c_{12}$

$Q_{66} = 1/2(c_{11}-c_{12}) = c_{44}$

$c_{11} = E / (1 - \upsilon^2)$ $\qquad$ $c_{12} = \upsilon E / (1 - \upsilon^2)$

$Q_{66} = c_{44} = E / 2 (1 + \upsilon)$

Anisotropic solid:

3D $\Rightarrow$ 21 constants ; **2D** $\Rightarrow$ 6 independent constants

Crystal symmetry reduces the number of independent constants:

In cubic crystals, 3 independent elements:

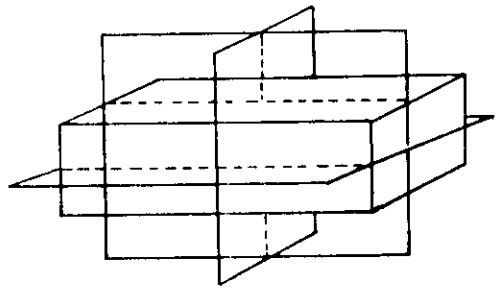
$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{44}\end{bmatrix} \begin{bmatrix}\epsilon_1\\ \epsilon_2\\ \epsilon_3\\ 2\epsilon_4\\ 2\epsilon_5\\ 2\epsilon_6\end{bmatrix}$$

In hexagonal crystals:

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0\\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{66}\end{bmatrix} \begin{bmatrix}\epsilon_1\\ \epsilon_2\\ \epsilon_3\\ 2\epsilon_4\\ 2\epsilon_5\\ 2\epsilon_6\end{bmatrix}$$

or $(c_{11}-c_{12})/2$

Orthotropic materials:



$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \tau_{23}\\ \tau_{13}\\ \tau_{12}\end{bmatrix} = \begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0\\ c_{12} & c_{22} & c_{23} & 0 & 0 & 0\\ c_{13} & c_{23} & c_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{55} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{66}\end{bmatrix} \times \begin{bmatrix}e_1\\ e_2\\ e_3\\ \gamma_{23}\\ \gamma_{13}\\ \gamma_{12}\end{bmatrix}$$

Special conditions

Transverse isotropy		Isotropic
$1 \neq 2, 3$	$3 \neq 1, 2$	$c_{11} = c_{22} = c_{33}$
$c_{22} = c_{33}$	$c_{11} = c_{22}$	$c_{12} = c_{13} = c_{23}$
$c_{12} = c_{13}$	$c_{23} = c_{13}$	$c_{44} = c_{55} = c_{66} = \frac{1}{2}(c_{11}-c_{12})$
$c_{44} = \frac{1}{2}(c_{22}-c_{23})$	$c_{44} = c_{55}$	
$c_{66} = c_{55}$	$c_{66} = \frac{1}{2}(c_{11}-c_{12})$	

1.11. ISOTROPIC SOLIDS. DEDUCTION OF RELATION BETWEEN ELAST. CONSTANTS

Suppose only $\epsilon_{11} \neq 0$, $\epsilon_{ij} = 0$ for $i \neq j$ or $i = j \neq 1$

Then:

$$\sigma_{11} = c_{11} \epsilon_{11}$$

$$\sigma_{22} = \sigma_{33} = c_{12} \epsilon_{11} = \frac{c_{12}}{c_{11}} \sigma_{11}$$

Now rotate the coordinate systems 45° about the 3 axis:

$$T_{ij} = \begin{vmatrix} \sqrt{2}/2 & \sqrt{2}/2 & 1 \\ -\sqrt{2}/2 & \sqrt{2}/2 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

$$\epsilon'_{12} = T_{11} T_{21} \epsilon_{11} = 1/2 \epsilon_{11}$$

$$\sigma'_{12} = (c_{11} - c_{12}) \epsilon'_{12}$$

But due to isotropy:

$$\sigma'_{12} = 2 c_{44} \epsilon'_{12}$$

$$\Rightarrow \qquad c_{44} = (c_{11} - c_{12}) / 2$$

Two independent constants for isotropic medium!

Anisotropy ratio in cubic crystals:

$$A = 2 c_{44} / (c_{11} - c_{12})$$

EXERCISES:

Find the relation between the following pairs of constants defining Hooke's law in isotropic solids:

1) Lame constant: λ and shear modulus: μ ;

where $\lambda = c_{12}$, $\mu = c_{44}$

2) Compressibility K and shear modulus: μ ;

where $-K = (\Delta V/V) / p$ is the ratio of the negative of the dilation: $\Delta V / V = \epsilon_{11} + \epsilon_{22} + \epsilon_{33}$ to the pressure:

$p = - 1/3 \ (\sigma_{11} + \sigma_{22} + \sigma_{33})$

3) Young's modulus E and Poisson's ratio υ ;

where E and υ are defined in an uniaxial tension test as being E the ratio of the simple tensile stress to strain and υ the ratio of transverse contraction to elongation.

EIGENSTRAINS

2.1. EIGENSTRAINS

(T. Mura: "Micromechanics of Defects in Solids" (1987) Martinus Nijhoft Pub., Dordrecht).

Eigenstrains: generic name of non-elastic strains, such as thermal expansion, phase transformation, initial strains, plastic strains and misfit strains.

Eigenstress: self-equilibrated internal stresses caused by one or several of these eigenstrains in bodies which are free from any other external force and surface constraint.

Examples of eigenstresses:

"Residual stress" remaining after fabrication or plastic deformation,

or

"Thermal stress" when thermal expansion is the cause.

A part Ω of the material has its temperature raised by ΔT:

$$\epsilon^*_{ij} = \delta_{ij}\, \alpha\, \Delta T\, H$$

H: Heavyside function: $H(\underline{x}) = 1 \quad (x \in \Omega)$

$H(\underline{x}) = 0 \quad (x \notin \Omega)$

α: Thermal expansion coefficient

δ: Kronecher delta

Eigenstrain concept can be used to solve:

Inclusion field.

$\underline{\epsilon}^*$ defined in a finite subdomain Ω

Inhomogeneity:

$c^* \neq c$ in Ω

Those cover the description of the elastic field of:

Point defects

Precipitates

Martensites

Cracks

Defects associated to a set of volume forces.

Classical papers:

J.D. Eshelby

Solid State Physics 3, Eds. F. Seitz and D. Turnbull, Academic Press (1956), 79-144.

Proc. Roy. Soc. A241 (1957), 376-396.

Proc. Roy. Soc. A252 (1959), 561-569.

Periodic Eigenstrains

$$\epsilon^*_{ij}(\underline{x}) \quad \epsilon^*_{ij}(\xi) \exp(i\,\xi \cdot \underline{x})$$

Used for modelling:

Coherent inclusion of a new phase

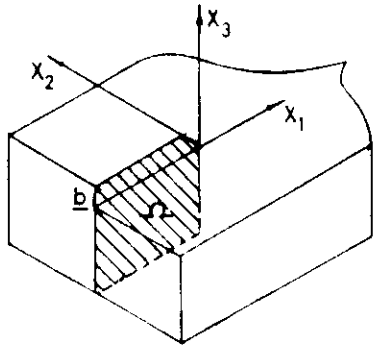
Distribution of dislocations

Straight dislocation:

Screw:

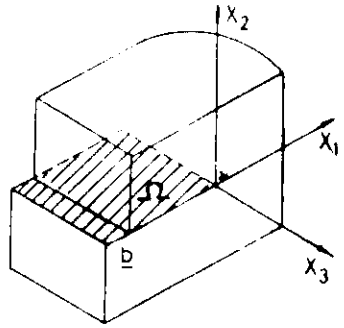
$$\epsilon^*_{23}(\underline{x}) = 1/2\ \delta(x_2)\ H(-x_1)$$

$$H(-x_1) = \begin{cases} 1 & x_1 < 0 \\ 0 & x_1 > 0 \end{cases}$$



Edge:

$$\epsilon^*_{31}(\underline{x}) = 1/2\ b\,\delta(x_2)\ H(-x_1)$$



Defects associated to a violation of compatibility conditions.

2.2. ELASTIC FIELD CAUSED BY EIGENSTRAINS

Strain

$$\epsilon_{ij} = e_{ij} + \epsilon^*_{ij}$$

e: elastic strain

Where

$$e_{ij} = 1/2\ (u_{i,j} + u_{j,i})$$

where

$$u_{i,j} = \partial u_i / \partial x_j$$

and the elastic stress:

$$\sigma_{ij} = C_{ijkl}\, e_{kl} = C_{ijkl}\,(\epsilon_{kl} - \epsilon^*_{kl})$$

Equilibrium

$$\sigma_{ij,j} = 0 \qquad (i = 1, 2, 3)$$

and free external surface

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

$$\Downarrow \quad \text{imply}$$

$$\sigma_{ij,j} = C_{ijkl}\,(\epsilon_{kl,j} - \epsilon^*_{kl,j}) = 0$$

$$C_{ijkl}\, u_{k,lj} = C_{ijkl}\, \epsilon^*_{kl,j}$$

$$\sigma_{ij}\, n_j = C_{ijkl}\,(\epsilon_{kl} - \epsilon^*_{kl})\, n_j = 0$$

$$C_{ijkl}\, u_{k,l}\, n_j = C_{ijkl}\, \epsilon^*_{kl}\, n_j$$

2.3. STATIC GREEN FUNCTION IN A CONTINUUM SOLID

If a body force:

$$f_i(\underline{x}) = \delta_{im}\,\delta(\underline{x} - \underline{x}')$$

is applied at $\underline{x}' = \underline{x}$ in a direction m, the displacement field will have the components:

$$(G_{1m}(\underline{x} - \underline{x}'),\quad G_{2m}(\underline{x} - \underline{x}'),\quad G_{3m}(\underline{x} - \underline{x}'))$$

such that

$$c_{ijkl}\,G_{km,lj}(\underline{x} - \underline{x}') + \delta_{im}\,\delta(\underline{x} - \underline{x}') = 0$$

Therefore,

Green function: $G_{ij}(\underline{x} - \underline{x}')$ is the x_i component of displacement at a point $\underline{x}$ when a body force in the x_j direction is applied at point $\underline{x}'$.

2.4. PERIODIC SOLUTION

$$\varepsilon^{*}_{ij}(\underline{x}) = \bar{\varepsilon}^{*}_{ij}\,\exp(i\,\underline{\xi}\cdot\underline{x})$$

or

$$u_i(\underline{x}) = \alpha_i\,\exp(i\,\underline{\xi}\cdot\underline{x})$$

Both $\bar{\varepsilon}$ and α may be complex numbers.

If

$$c_{ijkl}\,u_{k,lj} = c_{ijkl}\,\varepsilon^{*l,j}_{k}$$

$$c_{ijkl}\,\alpha_k\,\xi_l\,\xi_j = -i\,c_{ijkl}\,\bar{\varepsilon}^{*}_{kl}\,\xi_j$$

If we call

$$c_{ijkl}\,\xi_i\,\xi_j = K_{ik}$$

$$-i\,c_{ijkl}\,\bar{\varepsilon}^{*}_{kl}\,\xi_j = X_i$$

$$K_{ik}\,\alpha_k = X_i \qquad \text{6 linear equations for } i = 1, 2, 3$$

Solution:

$$\alpha_i(\underline{x}) = X_j\,N_{ij}(\underline{\xi}) / D(\underline{\xi})$$

N_{ij} cofactors of the matrix:

$$\underline{K}(\underline{\xi}) = \begin{matrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{matrix}$$

$D(\xi)$ is the determinant of $K(\xi)$; $K(\xi)$ is called the Green-Christoffel matrix.

Applying the periodic approach to Fourier transform the equation for the Green function, one obtains:

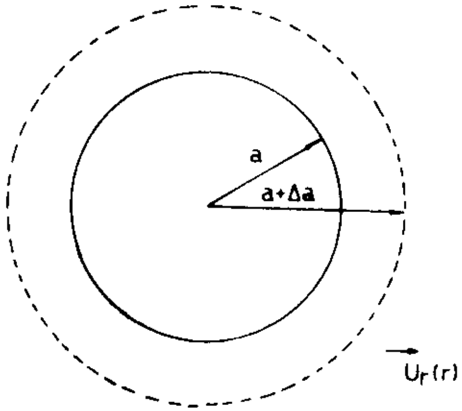
$$G_{ij}(\mathbf{x} - \mathbf{x}') = (2\Pi)^{-3} \int_{-\infty}^{\infty} N_{ij}(\boldsymbol{\xi})\, D^{-1}(\boldsymbol{\xi}) \exp(i\, \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{x}'))\, d\boldsymbol{\xi}$$

3. ESHELBY'S INCLUSION

3.1. ESHELBEY'S INCLUSION

Rigid Spherical Inclusion

Problem: to introduce in a spherical hole of radius a within an infinite elastic isotropic solid a **rigid** sphere of radius "a + Δa":



Find $\mathbf{u}(r)$

$u_\theta = 0 \rightarrow |\mathbf{u}(r)| = u_r(r)$

By using $e_r = du/dr \qquad e_\theta = u/r$

and

$$e_r = (1/E)(\sigma_r - 2\nu\,\sigma_\theta)$$

$$e_\theta = (1/E)[(1-\nu)\,\sigma_\theta - \nu\,\sigma_r]$$

It results

$$u_r(r) = C_1 \frac{(1-2\nu)}{E}\, r + C_2 \frac{(1+\nu)}{2E} \frac{1}{r^2}$$

Now we apply boundary conditions

$$u_r\ (r \to \infty) = 0 \quad \Rightarrow \quad C_1 = 0$$

$$u_r\ (r = a) = \Delta a \quad \Rightarrow \quad C_2 = \Delta a \frac{2a^2 E}{(1 + \nu)}$$

HOMEWORK

1.1) Find explilcit expressions for $\underline{\sigma}$, $\underline{\varepsilon}$ field.

1.2) Find the volume expansion

$$\Delta V(r) = \int_{S_r} u_r \cdot dS$$

where S_r is a spherical surface at a radius r.

Does ΔV depend on r?

1.3) Find the local volume expansion $\delta V / V_0 = 1/3 \ \mathrm{Tr}\ \underline{\varepsilon}$

1.4) Find $\underline{u}$ as a function of ΔV.

1.5) Find the pressure in the inserted material.

1.6) Find the "eigenstrain" ε*

1.7) Find the elastic energy stored in the solid.

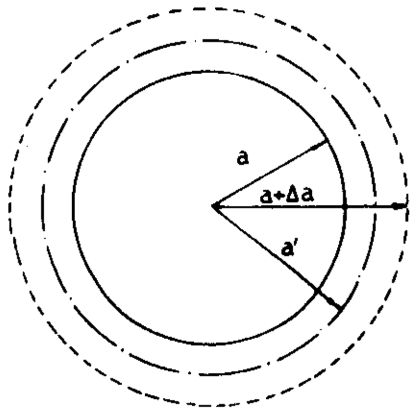
3.2. ELASTIC INCLUSION

Problem: to introduce in a spherical hole of radius "a" within an infinite elastic isotropic solid an elastic sphere of radius "a + Δa" and elastic constants E*, ν*.

Previous solution is still valid for spherical geometry and centrosymmetric expansion field:

$$u_r(r) = \frac{(1 - 2\nu)}{E} C_1 r - \frac{C_2}{2E} \frac{(1 + \nu)}{r^2}$$

However, the original hole expands now into a larger one of radius a'. That is, the elastic sphere contracts from a + Δa to a' and the hole wall expand from a to a'.



Two regions must be considered; it results:

for $r \leq a'$

$$u_r^I(r) = \frac{(1-2\nu^*)}{E} C_1 r$$

for $r \geq a'$

$$u_r^{II}(r) = -\frac{C_2}{2E} \frac{(1+\nu)}{r^2}$$

Boundary conditions at a' (careful: not an original point at undistorted solid! but easy to understand):

$$a + \Delta a + u_r^I \Big|_{r=a'} = a + u_r^I \Big|_{r=a'}$$

original radius of solid sphere — original radius of hole wall

Equilibrium:

$$\sigma_r^I \Big|_{r=a'} = \sigma^{II} \Big|_{r=a'}$$

3 unknown C_1, C_2, a' !

If $a' = a = a + \Delta a$ it results:

$$C_2 = \frac{(2 E E^*) \Delta a a^2}{[E^*(1+\nu) + 2E(1-2\nu^*)]}$$

$$C_1 = -\frac{(2 E E^*) \Delta a}{a [E^*(1+\nu) + 2E(1-2\nu^*)]}$$

HOMEWORK

2.1) Find explicit expressions for $\underline{\sigma}$, $\underline{\varepsilon}$.

2.2) Find the volume expansion at $r \to \infty$.

2.2.1) for $E^* \to \infty$

2.2.2) for $E^* \to 0$

2.3) Find the elastic energy stored in the solid.

2.4) Solve the problem of a spherical inclusion in a finite elastic sphere.

See how the condition of a stress-free external surface is equivalent to impose a distortion field

$$\underline{u} = \underline{u}^\infty + \underline{u}^I$$

where u^∞ is the solution for the infinite body. In turn, the "eigenstrains" can be considered to be

$$\varepsilon^* = \varepsilon^{*\infty} + \varepsilon^{*I}$$

Find explicitly the total strain, separate it into elastic and eigenstrain.

3.3. SPHERICAL CAVITY

The solution of the problem 1.7 above is:

Energy density:

$$\omega(r) = 2/3\ G(2a^2\ \Delta a\ /\ r^3)^2$$

The stored elastic energy:

$$U_{elast} = 8\Pi\ G\ a\ \Delta a^2$$

where $G = E\ /\ 2\ (1+\nu)$ shear modulus

To create the cavity, an energy:

$$U_\gamma = 4\Pi\ (a + \Delta a)^2\ \gamma$$

has to be provided. Where γ: surface energy.

In equilibrium:

$$\partial(U_{elast} + U_\gamma)\ /\ \partial(\Delta a) = 0 \quad \rightarrow$$

$$\Delta a = -\ a\ /\ (1 + 2\ G\ a/\gamma) \approx -\ \gamma\ /\ 2G$$

3.4. VACANCY FORMATION ENERGY

From the above section, one can find that the energy to create a vacancy is approximately:

$$U_f^v \approx 4\Pi\ a^2\ \gamma - 2\Pi\ a\frac{\gamma^2}{G} + \Pi\frac{\gamma^3}{G^2}$$

where a corresponds now to a lattice parameter. The first term coresponds to the energy of creating the spherical hole; assuming: $\gamma = 0.1$ eV / Å^{-2} , a = 1.5 Å it results $4\Pi\ a^2\ \gamma = 2$ eV. The second and third term contain the elastic relaxation due to the inward displacement of the solid. These terms reduce the energy to approximately 2/3 of the above value.

See "Defects and Radiation Damage" by Thompson for further discussion along this line.

4. POINT DEFECTS

4.1. POINT DEFECTS IN SOLIDS

Useful thermodynamics review:

P, V, T: thermodynamic parameters (Pressure, Volume, Temperature)

$f(P, V, T) = 0$: Equation of state.

State functions:

Internal energy: U

Enthalpy $H = U + PV$

Free energy: $F = U - ST$

Gibbs energy: $G = F + PV = H - ST$

where S: entropy.

We shall in general be interested in systems in equilibriuum at T and P constants. That is, we shall look for a minimum of the Gibbs energy.

We now want to introduce the concept of configurational entropy for a population of defects.

Let us first treat as an example the case of an ideal gas; equation of state:

$$P V = n R T$$

Isothermal expansion:

$$dq = - dw = P\,dV$$

q: heat , w: work

The entropy changes from a state 1 to a final 2:

$$S_2 - S_1 = \int_{V_1}^{V_2} \frac{dq}{T} = n R \ln \frac{V_2}{V_1}$$

Suppose now that we have separate containments of different ideal gases. A given gas α occupies a volume V_α. We allow this mixture by communicating the containments. The adiabatic entropy change will be:

$$S_c = - R \sum_\alpha n_\alpha \ln\left(\frac{V_\alpha}{V}\right) = - R \sum_\alpha n_\alpha \ln c_\alpha$$

Where n_α: number of moles of α

$$V = \sum_\alpha V_\alpha$$

4.... CONFIGURATIONAL ENTROPY FOR POINT DEFECT

$$S = k_B \ln \pi$$

k_B: Boltzman constant

π: multiplicity of configuration

Suppose that in the solid there are a total number of atomic/defect sites:

$$N = \sum_\alpha N_\alpha$$

occupied by N_α atoms/defects of type α.

$$\pi = \prod_\alpha \frac{N}{(N_\alpha)}$$

Now, $\ln (N!) = N \ln N - N$ Stirling relation

$$S_c = -k_B \sum_\alpha N_\alpha \ln \left(\frac{N_\alpha}{\sum_\alpha N_\alpha} \right) = k_B \sum_\alpha N_\alpha \ln c_\alpha$$

n moles of defects (vacancies, interstitials, etc.) in thermal equilibrium:

$$G = G_o + ng - S_c T$$

g: Gibbs energy to create <u>one</u> defect in an otherwise perfect lattice. $g = h - s T$

G_o: perfect lattice energy

Equilibrium:

$$\partial G / \partial n = \mu = 0 \qquad (\mu: \text{chemical potential})$$

$$\partial G / \partial n = g + R T \ln c = 0$$

Equilibrium:

$$c = \exp (- g / R T)$$

5. LATTICE STATICS

Adiabatic interatomic potentials

Harmonic limit: Green function, Kanzaki forces

Lattice statics vs elasticity

Potential defects

Dislocations

Recommended reading:

G Leibfried, N. Breuer; "Point Defects in Metals I", Springer Tracts in Modern Physics 81 (1978). Springer Verlag, Berlin - Heidelberg - New York.

P.H. Dederichs, R. Zeller; "Point Defects in Metals II", Dynamical Properties of Point Defects in Metals. Springer Tracts in Modern Physics 87 (1980). Springer Verlag, Berlin - Heidelberg - New York.

5.1. ADIABATIC INTERATOMIC POTENTIAL IN A SOLID

Generally the energy of a solid $U = U(\underline{r}^l, \underline{r}^e)$ depends on $\underline{r}^l$, the position of the atoms, and $\underline{r}^e$, the electron location (or distribution), for every atom l and electron e.

The adiabatic approximation stands for $\underline{r}^e$ to follow instantaneously the atoms l accomodating to a minimum electronic contribution to the energy.

This approximation allows to define an energy function:

$\Phi(\underline{r}^1 \ldots \underline{r}^l \ldots \underline{r}^N$ for the N atoms of the solid.

Φ must be translational and rotational invariant.

$$\Phi(\ldots \underline{r}^m \ldots) = \Phi(\ldots \underline{\tilde{r}}^m \ldots)$$

where

$$\underline{\tilde{r}}^m = \underline{D}\,\underline{r}^m + \underline{T}\xi$$

being:

$\underline{D}$: rotation matrix

$\underline{T}$: translation vector

$$\tilde{x}_i^m = x_i^m + T_i + \omega_{ik}\, x_k^m$$

$$D_{ik} = \omega_{ik} \quad \text{and} \quad \omega_{ik} = -\omega_{ki}$$

We can perform a series expansion of:

$$\Phi\ (\ldots \underline{\mathcal{L}}^{m} \ldots) \;-\; \Phi\ (\ldots \underline{\mathcal{L}}^{m} \ldots) + \sum_{m} (\omega_{ik}\, x_k^{m} + \ldots)\ \Phi_i^{m}$$

where

$$\Phi_i^{m} \;-\; \frac{\partial \Phi}{\partial x_i^{m}}$$

Translational invariance implies:

$$\sum_{m} [-\ \Phi_i^{m}] \;-\; 0$$

(null forces on an atom)

and rotational invariance:

$$\sum_{m} \omega_{ik}\, x_k\ [-\ \Phi_i^{m}] \;-\; 0$$

that is

$$\sum_{m} x_k^{m}\, \Phi_i^{m} \;-\; \sum_{m} x_i^{m}\, \Phi_k^{m}$$

(null torques)

5.2. HARMONIC APPROXIMATION

Assume the displacement of atom m from perfect lattice to be $\underline{s}^{m}$ and series expand the

$$\Phi\ (\ldots, \underline{R}^{m} + \underline{s}^{m}, \ldots) \;=\; \Phi\ (\ldots, \underline{R}^{m}, \ldots) + \Phi_i^{m}\ (\ldots, \underline{R}^{m}, \ldots)\ s_i^{m} +$$
$$+\ 1/2\ \Phi_{ik}^{m}\ (\ldots, \underline{R}^{m}, \ldots)\ s_i^{m}\ s_k^{n} +$$
$$+\ \text{higher order terms}\ \}\ \text{Harmonic}$$

approximation implies neglecting these terms.

We have defined: Force constant matrix:

$$\Phi_{ik}^{mn} \;-\; \frac{\partial}{\partial x_i^{m}}\ \frac{\partial}{\partial x_k^{n}}\ \Phi$$

(Note that bellow, the alternative notation $\Phi_{i\ k}^{m\ n} \;=\; \Phi_{ik}\ (l^{m},\ l^{n})$ is also used)

The above definition implies:

$$\Phi_{ik}^{mn} \;-\; \Phi_{ki}^{nm}$$

While, translational invariance

$$\Downarrow$$

$$\sum_{n} \Phi_{ik}^{mn} \;-\; \sum_{m} \Phi_{ik}^{mn} \;-\; 0$$

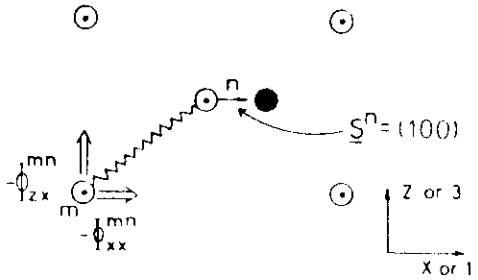
and rotational invariance

$$\Downarrow$$

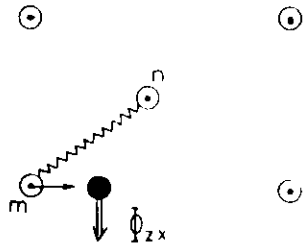
$$\Phi_{ik}^{mn}\, x_l^{n} \;-\; \Phi_{il}^{mn}\, x_k^{n}$$

Force constants are called coupling parameters or force or spring constants.

- $\Phi^{m\ n}_{i\ k}$ is the internal force on m in direction i if only atom n is displaced by unit length in direction k and all other atoms remain in their equilibrium position.



It is also the contribution of spring m-n to self restoring force if only m is displaced:

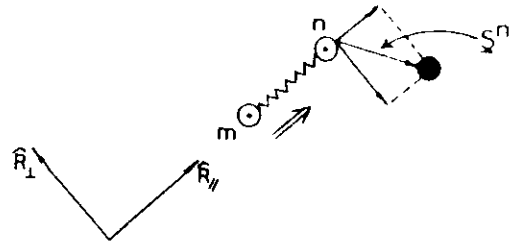


See that in a rotated coordinate system with an axis parallel to the vector $\underline{x}_{//} = \underline{x}^m - \underline{x}^n$:

$$\Phi^{m\ n}_{i\ j} = D_{ik}\ D_{jk}\ \Phi^{m\ n}_{k\ l}$$

$\Phi^{m\ n}_{//\ //}$ is the internal force or the contribution of the spring parallel to the vector joining both atoms.

For a simple spring of constant k between m and n :



$$\hat{R}_{//} = (\underline{x}^m - \underline{x}^n) \ / \ |\underline{x}^m - \underline{x}^n|$$

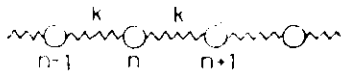
$$\underline{s}^n = (\underline{s}^n \cdot \underline{R}_{//})\ \hat{R}^{//} + (\underline{s}^n \cdot \underline{R}_\perp)\ \hat{R}_\perp = s^n_{//}\ \hat{R}_{//} + s^n_\perp\ \hat{R}_\perp$$

Longitudinal spring k between atoms m and n : the force is in the spring direction $\hat{R}_{//}$ and proportional to the elongation in the spring direction.

$$\Phi = \Phi_o + 1/2\ k\ (s^n_{//} - s^m_{//})^2$$

$$\Phi^{m\ n}_{i\ k} = - k\ (\hat{R}_{//})_i\ (\hat{R}_{//})_k$$

Lineal chain (one dimensional harmonic oscillator)



Restoring force:

$$F_x^n = -k\,(s_x^n - s_x^{n-1}) - k\,(s_x^n - s_x^{n+1}) =$$
$$= -2k\,s_x^n + k\,s_x^{n-1} + k\,s_x^{n+1}$$

$$\Phi = \Phi_o + \sum_n \frac{1}{2} F^n s^n =$$
$$= \Phi_o + \sum_n k(s^n)^2 + \frac{1}{2} k\,s^n s^{n-1} + \frac{1}{2} k\,s^n s^{n+1}$$

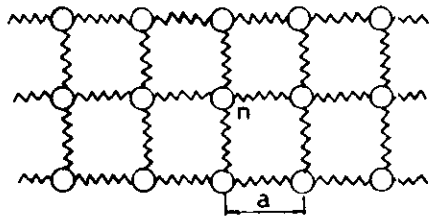
5.3. BOUNDARY CONDITION

Example, periodic boundary or Bon Von Karman condition $s^N = s^1$

Two dimension cubic lattice:

$n = (n_x, n_y)$

$m = (m_x, m_y)$



$$F_x^n = -k\,(s_x^{(n_x,n_y)} - s_x^{(n_x-1,n_y)}) - k\,(s_x^{(n_x,n_y)} - s_x^{(n_x+1,n_y)}) -$$
$$- k\,(s_y^{(n_x,n_y)} - s_y^{(n_x,n_y-1)}) - k\,(s_y^{(n_x,n_y)} - s_y^{(n_x,n_y+1)})$$

$$\Phi = \sum_n \frac{1}{2} k(\Delta r^n)^2$$

$$\Delta r^{nn'} = [(a+s_x^{n'}-s_x^n)^2 + (s_y^{n'}-s_y^n)^2]^{1/2} - a$$
$$n = (n_x, n_y) \qquad n' = (n_x+1, n_y)$$

$$\Phi - \Phi_o = \sum_{n,m} \frac{1}{2} k(\Delta r^{nm})^2 \qquad k_\parallel = k\ ,\ k_\perp = 0$$

$$\Delta r^{nn'} = (s_x^{n'} - s_x^n) + \frac{(s_y^{n'} - s_y^n)^2}{a} + \frac{(s_x^{n'} - s_x^n)^2}{a}$$

$$F_x^n = \frac{\partial(\Phi - \Phi_o)}{\partial s_x^n}$$

5.4. DYNAMICS OF AN ASSEMBLY OF ATOMS (lattice dynamics)

Time "t" is introduced.

Assume $s_\alpha^m(t) \quad s_\alpha^{0m} e^{i\omega t}$

$$\Delta\Phi = 1/2\ \Phi_{\alpha\beta}^{m\,n}\, s_\alpha^m\, s_\beta^n$$

$$F_\alpha^m = \Phi_{\alpha\beta}^{m\,n}\, s_\beta^n \quad \rightarrow \quad \Phi_{\alpha\beta}^{m\,n}\, s_\beta^{0n}\, e^{i\omega t}$$

$$F_\alpha^m = M^m \ddot{s}_\alpha^m \quad M^m \omega^2 s_\alpha^{0m} e^{i\omega t}$$

Eigenvalues, eigenvectors of Φ:

$$\underline{S}^\nu = \nu\rangle \qquad \nu = 1, \ldots, 3N$$

$$\Phi\ \underline{S}_\nu = \Phi^\nu\ \underline{S}^\nu \quad \rightarrow \quad \Phi^\nu / M^m = (\omega_\nu)^2$$

Translational, rotational invariance $\rightarrow \Phi^\nu = 0 \qquad \nu = 1,6$

Stability $\Phi^\nu > 0 \qquad \nu = 7, \ldots, 3N$

5.5. FOURIER TRANSFORM OF FORCE CONSTANT MATRIX

Lattice symmetry implies:

$$\Phi_{\alpha\beta}^{m\,n} = \Phi_{\alpha\beta}^{m-n} = \Phi_{\alpha\beta}^{(m-n),0}$$

where now $\underline{m}$ and $\underline{n}$ stand for position vector of the atoms m and n and $-\underline{m}$, $-\underline{n}$ for an atom at $-\underline{m}$, $-\underline{n}$.

Eigenvalues and eigenvectors:

If we take a vector in space of dimension 3 (while $\underline{R}^m$ are vectors in a 3N dimension space and $\Phi_{\alpha\beta}^{m\,n}$ are matrix of 3N x 3N).

$$\Phi_{\alpha\beta}^{m\,n} A_\beta \exp(i\underline{k}\cdot\underline{R}^n) = \Phi_{\alpha\beta}^{(n-m),0} A_\beta \exp\{i\underline{k}\cdot[(\underline{R}^n-\underline{R}^m)+\underline{R}^m]\} =$$

$$= \sum_{\underline{h}} \Phi_{\alpha\beta}^{\underline{h}}\,(-i\underline{k}\cdot\underline{h})\, A_\beta \exp(i\underline{k}\cdot\underline{R}^m)$$

We obtain a 3 x 3 matrix $\rightarrow \dot{\Phi}_{\alpha\beta}(k)$
(in reciprocal space)

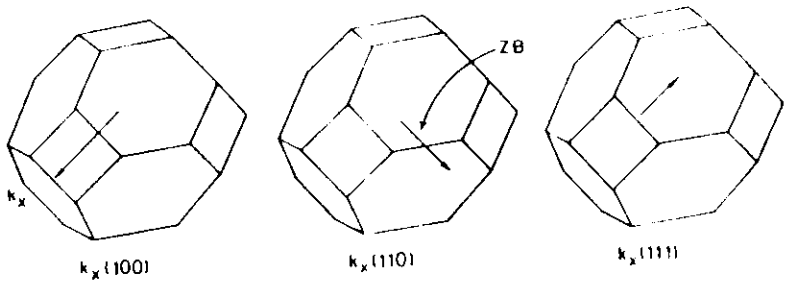
$\dot{\Phi}$ has eigenvalues $\Omega^2(k)$ and eigenvectors $\underline{e}(k)$

$$\rightarrow \quad \dot{\underline{\Phi}}(k)\ \underline{e}(k) = \Omega^2(k)\ \underline{e}(k)$$

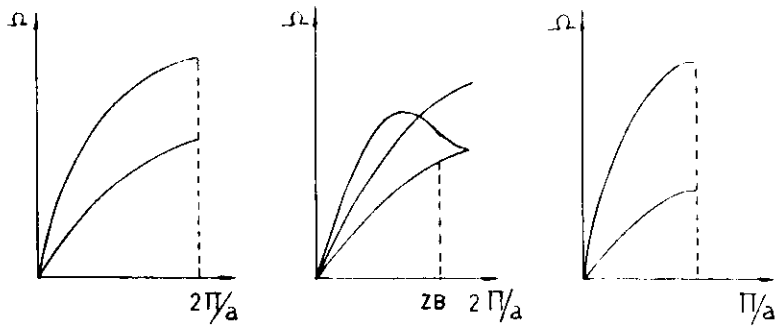
$$\rightarrow \quad \Phi^{mn}\ \underline{e}(\underline{k}) \exp(i\underline{k}\cdot R^n) = \Omega^2(k)\ e(k) \exp(i\underline{k}\cdot\underline{R}^m)$$

5.6. PHONON DISPERSION

Brillouin zone (in reciprocal space)



Dispersion curves



5.7. LATTICE STATICS

We can now go back to **lattice statics**.

Assume a force $\underline{K}^n$ is applied on an atom n

$$\Phi = \Phi_o - K_i^n s_i^n + \frac{1}{2} \Phi_{ik}^{nm} s_i^m s_k^n + \text{higher order terms}$$

In equilibrium

$$\frac{\partial \Phi}{\partial s_i^n} = 0$$

for every i, m

$$- K_i^n = \sum_{m \neq n} \Phi_{ik}^{nm} s_k^m - \left(\sum_{m \neq n} \Phi_{ik}^{nm}\right) s_k^n$$

$$0 = \sum_{m \neq 1} \Phi_{ik}^{1m} s_k^m - \left(\sum_{m \neq 1} \Phi_{ik}^{1m}\right) s) \frac{1}{k}$$

Where equilibrium conditions for ϕ are explicitly used.

The above is a system of 3N lineal equations. It can be solved if the 3N x 3N matrix:

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

is found. $\underline{G}$ is called the lattice Green function.

The solution for the displacements:

$$s_i^n = G_{ik}^{nn} K_k^n$$

(Note: G is in fact a (3N-6) x (3N-6) matrix due to the above conditions on ϕ and on the forces, this will be clear below).

Purpose: Find static configuration at defect lattice $\underline{s}^D$

$\underline{s}$: 3N coordinates vector (N: number of atoms)

Gibbs' Free Energy

$$\Delta G = G(\underline{s}^D) - G(\underline{s}^{P.L.})$$

$\underline{s}^D \rightarrow$ minimum of ΔG

$$G(\underline{s}) = V(\underline{s}) + kT\sum_{\alpha=1}^{3N} \ln \frac{\hbar\omega_\alpha}{kT} + pV(s)$$

$$V(\underline{s}^D) = V_{RP}(\underline{s}^{P.L.}) + \text{Terms depending on } (\underline{s}^D - \underline{s}^{P.L.}) + V_D(\underline{s}^D, \underline{x}^D)$$

(Perfect lattice) (ΔV_{RP}) (Potential energy due to the presence of the defect)

Harmonic approximation:

$$\Delta V_{RP} = \frac{1}{2} u_\alpha(l)\, \phi_{\alpha\beta}(l,l')\, u_\beta(l')$$

$$\phi_{\alpha\beta}(l,l') = \frac{\partial^2 V_{RP}}{\partial u_\alpha(l)\, \partial u_\beta(l')}$$

$$u(l) = s^l - s^{l\,0}_{Atom\,l}$$

5.8. DEFECTS

$$\Delta G = G(\underline{s}^D) - G(\underline{s}^{P.L.})$$

Harmonic approximation:

$$G(\underline{s}) = V(\underline{s}) + kT\sum_{\alpha=1}^{3N} \ln \frac{\hbar\omega_\alpha}{kT} + pV(\underline{s})$$

Vibration entropy:

$$s_1^v = k\sum_{\alpha=1}^{3N} \ln \frac{\omega_\alpha^0}{\omega_\alpha} - \frac{k}{2}\sum_{\alpha=1}^{3N} \ln \frac{(\omega_\alpha^0)^2}{(\omega_\alpha)^2} - \frac{k}{2} \ln \left[\frac{\Pi_{\alpha=1}^{3N} (\omega_\alpha^0)^2}{\Pi_{\alpha=1}^{3N} \omega_\alpha^2}\right]$$

$s_1 = s_1^e + s_1^v$
s_1^e : electronic contribution
$s_1^e << s_1^v$ for metals (except transition metals)

Now:

$$\underline{\mathbf{M}}\,\ddot{\underline{\mathbf{s}}} = \underline{\Phi}\,\Delta\underline{s} = \underline{\Phi}\,\underline{u}$$

$\underline{s}$: 3N vector of atomic coordinates $\underline{u}$: 3N displacements

Method for obtaining s_1^v:

$$\Pi_{\alpha=1}^{3N} M\omega_\alpha^2 = \det \Phi$$

$$g = V_D(\underline{l}+\underline{u}(\underline{l}) - \underline{x}^0(n)) + \frac{1}{2}\sum_{\substack{l,l'\\ i,j}} \Phi_{ij}(l,l')\, u_i(l)\, u_j(l') + V(\underline{l}+\underline{u}(l))$$

$$\frac{\partial g}{\partial u_i(l)} = 0 \quad \rightarrow$$

$$u_i(l) = G_{ij}(l,l')\, K_j(l')$$

where $\underline{G} = \underline{\Phi}^{-1}$ Green function

$$K_i(l) = -\partial[V_D(\underline{l}+\underline{u}(l)-\underline{x}^0(n)) + V(\underline{l}+\underline{u}(l))] / \partial u_i(l)$$

$$K_i(l) = F_i^0(l) + \mathcal{F}_i(l) + \frac{\partial K_i(l)}{\partial x_j(l')}\Big|_{\underline{u}=0} u_j(l')$$

Kanzaki force

$$g = V_D(\underline{l}-\underline{x}^0(n)) - \sum_{l,i} K_i(l)\cdot u_i(l) + \frac{1}{2}\sum_{\substack{l,l'\\ i,j}} \Phi_{ij}(l,l')\, u_i(l)\, u_j(l')$$

Dipole tensor:

$$u_i(l) = G_{ij}(l,l')\, K_j(l') =$$
$$= \Big(\sum_{l'} G_{ij}(l,0) + \sum_{l'} l'_k \frac{\partial G_{ij}(l,l')}{\partial x_k}\Big|_{l'=0} + \ldots\Big) K_j(l') =$$
$$= G_{ij}(l,o)\sum_{l'} K_j(l') + \frac{\partial G_{ij}(l,l')}{\partial x_k}\Big|_{l'=0}\sum_{l'} l'_k K_j(l') =$$
$$= G_{ij,k}(l,o)\, p_{kj}$$

$$\boldsymbol{P}\boldsymbol{k}_j = \sum_{l'} l'_k \boldsymbol{K}_j(l')$$

5.9. STATIC GREEN FUNCTION CALCULATION

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

$$K_\alpha(lk) = \sum_{\beta l'k'} \Phi_{\alpha\beta}(lk,l'k')\, u_\alpha(l'k')$$

$\mathbf{l} = l_1\hat{a}_1 + l_2\hat{a}_2 + l_3\hat{a}_3$: cell location

$\mathbf{k} = k_1\hat{a}_1 + k_2\hat{a}_2 + k_3\hat{a}_3$: atom location

Fourier transform:

$$\tilde{K} = K(k,\vec{q}) \;,\quad \tilde{\Phi} = \Phi(kk',\vec{q}) \;,\quad \tilde{u} = u(k,\vec{q})$$

For example:

$$\Phi_{ij}(kk',\vec{q}) = \sum_l \Phi_{ij}(lk,ok')\exp[-i\vec{q}\cdot\vec{r}(lk,o'k')]$$

where $\vec{r}(lk,ok') = \vec{r}(lk) - \vec{r}(ok')$

It is easy to prove:

$$\tilde{G}(lk,l'k') = G(kk',\vec{q}) = [\Phi(kk',\vec{q})]^{-1} = [\tilde{\Phi}(lk,l'k')]^{-1}$$

$$u_i(k,\vec{q}) = G_{ij}(kk',\vec{q})\, K_j(k',\vec{q})$$

(problem of 3N x 3N reduced to ($3\,k_{max}$ x $3\,k_{max}$))

If defect space is of dimension (3n) x (3n), same dimension implicit equation:

$$u_i(lk) = G_{ij}(lk,l'k')\, K_j(l'k')$$

5.10. GREEN FUNCTION CALCULATION METHOD

1)

$$\Phi\ (lk, l'k') \quad \rightarrow \quad \Phi\ (kk', \vec{q})$$

Can be obtained experimentally or explicitly from interatomic potential.

2)

$$\Phi\ (kk', \vec{q}) \quad \rightarrow \quad \Phi^{-1}\ (kk', q)$$

3)

$$G_{ij}\ (lk, l'k') = \frac{1}{N} \sum_{q} G_{ij}\ (kk', \vec{q})\ e^{i\vec{q}\,[\vec{r}(lk) - \vec{r}(l'k')]}$$

over N points in first Brillouin zone

Reduction of number of points in first Brillouin zone by symmetry arguments.

If

$$G\ (s\vec{q}) = g\ (s)\ G\ (\vec{q})\ g^{t}\ (s)$$

In cubic lattice:

$$G_{ij}(\vec{r}) = \frac{1}{N} \sum_{s \in P} \frac{2}{h_q} \sum_{\varepsilon}^{\pm} G_{ij}\ (s\vec{q})\ \cos\ (s\vec{q} \cdot \vec{r})$$

where inversion symmetry was explicitly included.

Group theory allows to write the addition explicitly.

5.11. LATTICE GREEN FUNCTION VS CONTINUUM

If

$$\vec{u}\ (\vec{r} + \vec{a}) - \vec{u}\ (\vec{r}) = a_i \frac{\partial \vec{u}}{\partial x_i} + \vec{e}$$

$$\vec{e} \rightarrow 0 \quad , \quad \vec{r} \rightarrow \infty$$

$$u_i\ (\vec{r}+\vec{a}) = u_i\ (\vec{r}) + e_{ij}\ a_j$$

$$E = E^{o} + \frac{1}{2}\ c_{ijkl}\ e_{ij}\ e_{kl} + \ldots$$

$$e_{ij} = \frac{1}{2}\ \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = \frac{1}{2N} \sum_{\alpha} \left[q_j^{\alpha}\ u_i\ (\vec{q}^{\alpha}) + k_i\ u_j\ (\vec{q}^{\alpha})\right]\ e^{i\vec{q}^{\alpha} \cdot \vec{r}}$$

$$E = E^{o} + \sum_{\alpha} c_{ijkl}\ q_i\ q_k\ e_j^{\alpha}\ e_l^{\alpha}$$

where $\vec{e}$ orthogonal plane waves.

Therefore,

$$\Phi\ (\vec{q}) \quad \rightarrow \quad \Delta\ (\vec{q})$$

$$\vec{q} \rightarrow 0$$

$$(\vec{r} \rightarrow \infty)$$

$$\Delta_{ij}\ (\vec{q}) = \rho^{-1}\ c_{ijkl}\ q_l\ q_k$$

$$G_c\ (\vec{r}) = \int \Delta^{-1}\ (\vec{q})\ e^{i(\vec{q}\vec{r})}\ d\vec{q}$$

5.12. VELOCITY OF ELASTICITY

Continuum

$$C_{ijkl}\, G''_{km,lj}\,(x,x') + \delta_{im}\,\delta\,(x-x') = 0$$

Point defect

Continuum

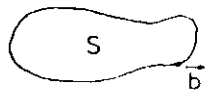
$$u_i\,(x) = G^{o}_{ij,k}\,(x,o)\; p_{jk}\,(o)$$

Lattice effects (non local elasticity)

$$u_i\,(x) = \sum_{l'} G''_{ij}\,(x,l')\; F^{o}_{j}\,(l')$$

Dislocation

Continuum



$$u_i\,(x) = -\int_S c_{ijkl}\, G_{km,l}\,(x',x)\; n_j\,(x')\; b_i\; dS\,(x')$$

However, defect core dominated by unharmonic terms.

5.13. POINT DEFECT AS A FORCE DISCONTINUITY

Formation energy:

$\dot{s}$: 3N coordinates vector of an ensamble of N atoms.

$$g = G'\,(\dot{s}^{defect}) - G\,(\dot{s}^{o}) =$$
$$= E'\,(\dot{s}^{defect}) - E\,(\dot{s}^{o}) + k\,T \sum_{\alpha} \ln \frac{\omega'_{\alpha}}{\omega^{o}_{\alpha}} + p\,(v' - v^{o})$$

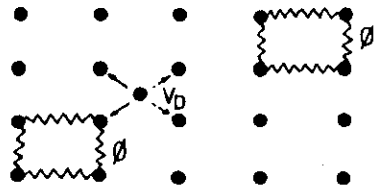
5.14. LATTICE STATICS

Quasi-Harmonic approximation:

$$\partial\, g \,/\, \partial\, u_i(l) \;\underset{\omega=0}{=}\; 0 \quad \rightarrow \quad u_i(l) = G_{ij}(l,l')\; K_j(l')$$

Green function: $\underline{G} = \underline{\Phi}^{-1}$

$$\Phi_{ij}(l,l') = (\partial^2 E\,(\dot{s}^{o})) \,/\, (\partial x_i(l)\; \partial x_j(l'))$$



Kanzaki forces:

$$\underline{K}_i(l) = (\partial(V_0 + V)) \,/\, (\partial u_i(l))$$

Elastic (continuum) limit:

$$u_i(l) = G_{ij,k}(l,o)\; P_{jk}(o) \quad \vec{l\to\infty} \quad u_i(l) = G^{el}_{ij,k}(l,o)\; P_{jk}$$

Dipole tensor:

$$P_{jk} = \sum_{l'} l'_j\, K_k(l')$$

Elastic limit is not bad, relatively near the center of distortion!

6.1 FROM HIGHLY HETEROGENEOUS MATERIAL AT MICRO-LEVEL TO AN EFFECTIVE HOMOGENEOUS ONE

Two approaches: either a fully empirical one or doing some theory.

Question:

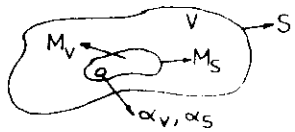
How to "homogenise"?

Several approaches in the literature:

D.R. Axelrad defines a "Probabilistic Micromechanics" (D.R.A. "Micromechanics of solids", Elsevier Sc. Pub., 1978).

One needs to find a self consistent relation between "macro" stresses, strains $\underline{\sigma}$, $\underline{\varepsilon}$ and "micro" internal variables ξ_α, ξ_α (K_α, e^*_α in our notation), where α stands for kind of microdefect.

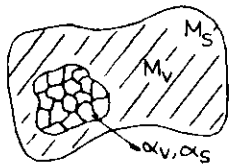
A Representative volume Element (RVE) of the body must be defined (S. Nemat-Nasser); Axelrad calls it a "mesodomain" within his probabilistic analysis.



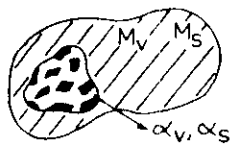
Macroscopic body: V, S

Particular mesodomain: M_V, M_S (M = 1, ...P)

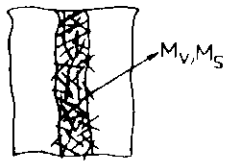
Microelement α_V, α_S (α = 1, ... N; N large)



Metallic grains



Two phase dispersed particles



Two dimensional network of fibers

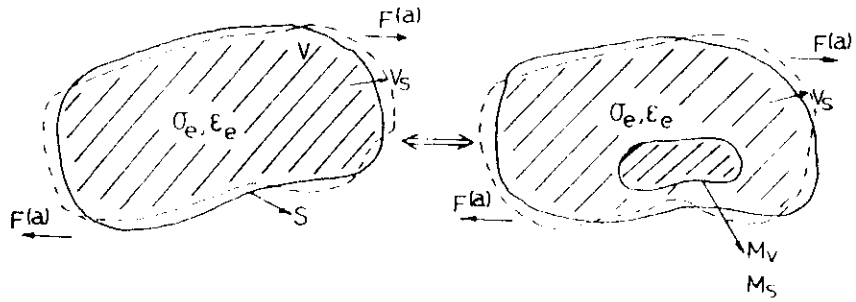
The mesodomains are "statistically" Representative Volume Elements (RVE).

The stresses and strains will be slowly varying from one RVE to an adjacent one.

Therefore, each RVE will reduce to a point in the continuum limit.

An "embedding procedure" (inspired in Eshelby's approach) must be adopted to ensure consistency.

The effective medium must be equivalent to a composed medium.



Recipe:

Solve the constitutive equation for σ_e, ε_e with boundary condition (b.c.) $F^{(a)}$ or $\underline{u}_S$ at S.

At every point M,

$$\sigma_{ij}(M) = \langle\sigma\rangle_{M_V} \quad , \quad \varepsilon_{ij}(M) = \langle\varepsilon\rangle_{M_V}$$

with b.c.:

$$(u_{M_S})_i = (\varepsilon_{ij})_{ij}\, x_j^o \quad x^o \text{ on } M_S$$

or

$$(T_{M_S})_i = (\sigma_{ij})_{ij}\, n_j \quad n \perp M_S \text{ on a perpendicular surface}$$

Within the previous recipe, at some level of the analysis one has to relate

$\underline{\underline{u}}$, $\underline{\underline{\varepsilon}}$ to internal variables f_α, ξ_α (K_α, ε_α^*

For α : point defects, see Hardy, V.K. Tewary and Bullough

α : dislocations, see a) statics: Bullough,

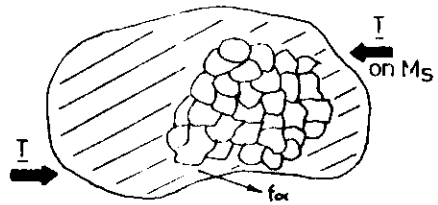
b) dynamics (climbing): Sarce, Harriague, Savino (additional material for lecture notes) and references in them.

6.2. OVERALL STRESSES IN GRANULAR MASSES (S. Nemat-Nasser)

RVE subjected on its boundary to uniform tractions T_i^o.

Forces at contact α: f_α

N: total number of contacts at M_V



To solve relation between T, consistent with $\langle\sigma\rangle$, and f_α one introduces an infinitesimal virtual displacement u_i which produces a virtual separation Δ_i^α at contact α.

$$\int_{M_V} T_i^o \, u_i \, dx \; - \; \sum_{\alpha=1}^{N} f_i^\alpha \, \Delta_i^\alpha$$

Since u_i can be chosen arbitrarily, take:

$$u_i \; = \; \phi_{ij} \, x_j \; + \; c_i$$

where ϕ_{ij} : arbitrary symmetric tensor
c_i : arbitrary constant vector
l_j^α : branch vector that connects centroids of the two granules

Compatible with u_i : $\Delta_i^\alpha \; = \; \phi_{ij} \, l_j^\alpha$

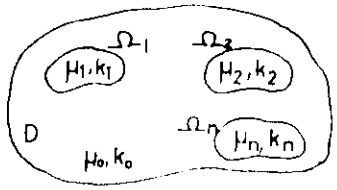
We arrive at:

$$\langle \sigma_{ij} \rangle \; - \; \frac{1}{2} \sum_{\alpha=1}^{N} \left(f_i^\alpha \, l_j^\alpha + f_j^\alpha \, l_i^\alpha \right)$$

6.3 AVERAGE ELASTIC MODULI OF COMPOSITE MATERIAL

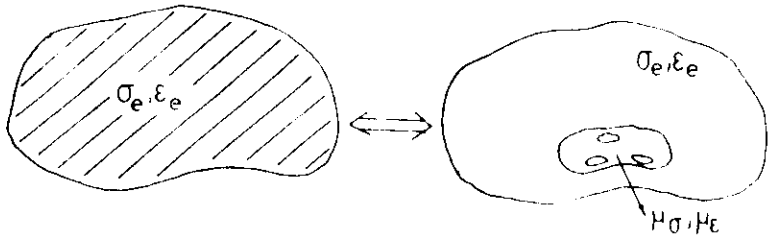
Assume the solid to be composed of a set of inhomogeneities (precipitates) with shear moduli $\mu_1 \dots \mu_n$ (caution: we have called it G in previous sections) and a matrix with μ_o (bulk modules $K_1 \dots K_n$, $K_o \dots K$

Volume fractions $c_o, c_1 \dots c_n$, $c_i = \Omega_i / D$



To avoid problems due to conditions at the surface assume $D \to \infty$ (infinite body).

Applied recipe for finding effective elastic constants:



The most simple approach, either:

homogeneous shear strain or homogeneous shear stress

$\epsilon_e = \langle \epsilon \rangle_D = E^0_{12} = \bar{\gamma} / 2$ $\sigma_e = \langle \sigma \rangle_D = \sigma^0_{12} = \mu_i \bar{\gamma}$

Voigt Reuss

Voigt Reuss

$\epsilon_e = \bar{\gamma} / 2$ $\sigma_e = \sigma^0_{12}$

this rigid internal strain this rigid internal stress

is imposed at every point

If c_r is the density of inclusions of type r (including c_o as the matrix)

$$(\bar{\mu}_i)_{12} = \mu_i \bar{\gamma} \qquad (\epsilon_i)_{12} = \frac{\sigma^0_{12}}{\mu_i}$$

$$(\sigma_o)_{12} = \langle \sigma \rangle = \sum_{r=0}^{n} c_r \mu_r \bar{\gamma} \qquad \bar{\gamma} = 2(\epsilon_o)_{12} = 2\langle \epsilon_{12} \rangle = \sum_{r=0}^{n} c_r \frac{\sigma_i}{\mu}$$

$$(\sigma_o)_{12} = \mu_o \bar{\gamma} \qquad \bar{\gamma} = 2(\epsilon_o)_{12} = \frac{(\sigma_o)_{12}}{\mu_o}$$

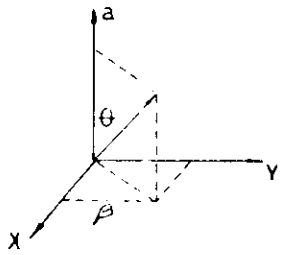
$$\mu_o^V = \sum_{r=0}^{n} c_r \mu_r \qquad \mu_o^R = \left(\sum_{r=0}^{n} \frac{c_r}{\mu_r}\right)^{-1}$$

$$K_o^V = \sum_{r=0}^{n} c_r K_r \qquad K_o^R = \left(\sum_{r=0}^{n} \frac{c_r}{K_r}\right)^{-1}$$

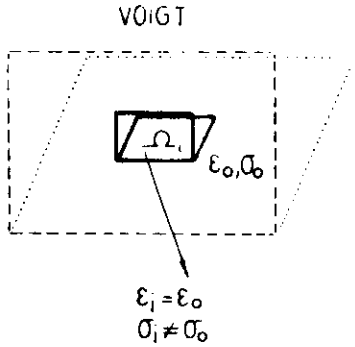
6.4 POLYCRYSTAL (without texture)

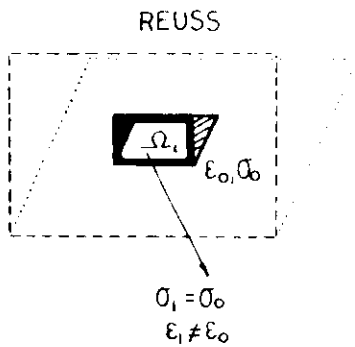
$$\bar{\mu}^{V} = \frac{1}{8} M^2 \int_0^{2\pi} d\beta \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} c_{1212} \, d\phi$$

$$\mu^{R} = \left(\frac{1}{2} M^2 \int_0^{2\pi} d\beta \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} s_{1212} \, d\theta\right)$$



However, Voigt and Reuss averages are not self consistent.





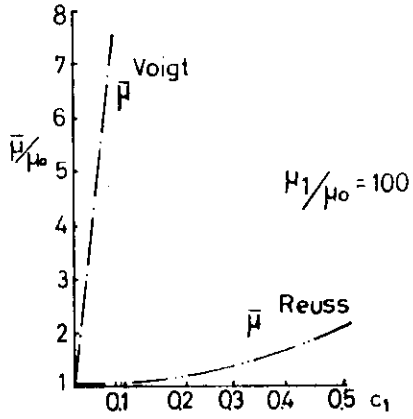
$\varepsilon_i = \varepsilon_o$

Compatibility condition at the the boundary i_s is not satisfied

$\sigma_i = \sigma_o$

Compatibility in strain is not satisfied

In a composite, it might give a large difference:

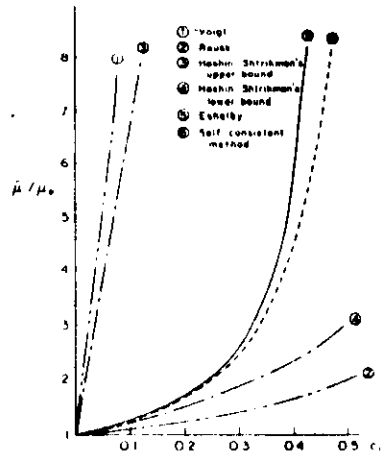


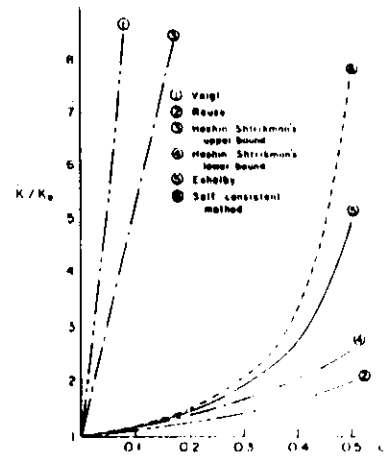
(T. Mura)

It can easily be proved: Voigt and Reuss averages are respectively upper and lower limits to elastic constants.

Same problem can be treated within a self-consistent approach.

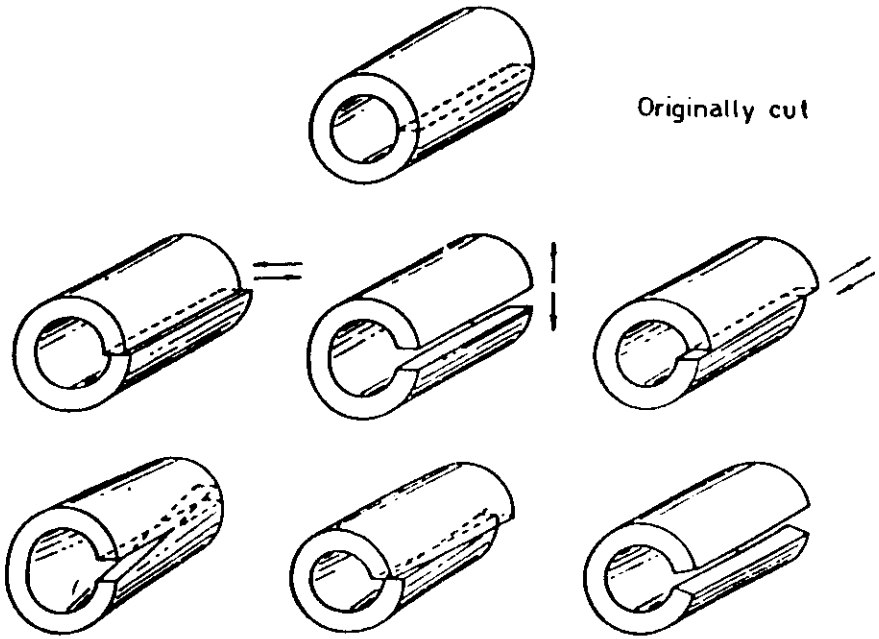
A summary of methods can be found in Mura's book ("Micromechanics of Defects in Solids, Rev.Ed., Martinus Nijhoff Publ., 1987)





7.1 STRAIGHT DISLOCATIONS

Volterra (1907) considered the elastic behavior of an homogeneous, isotropic cylinder deformed as:

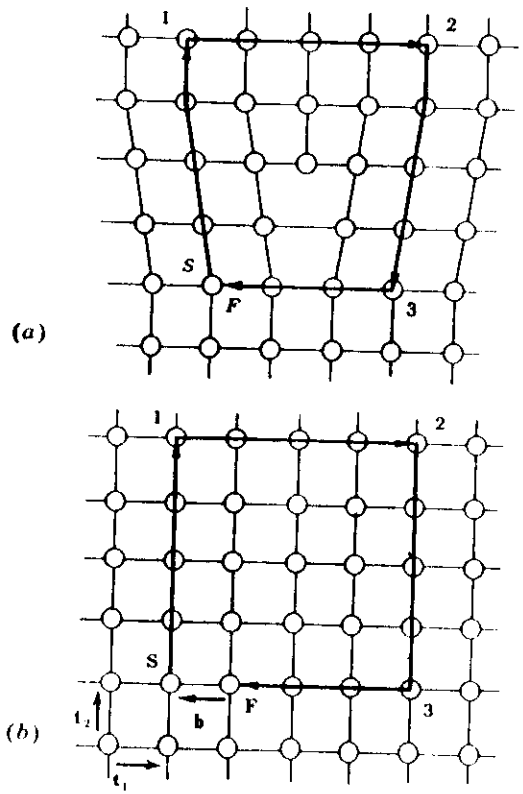


Ref.: J.P. Hirth and J. Lothe, Theory of Dislocations, Mc Graw Hill Book Company (1968).

7.2. BURGERS VECTOR

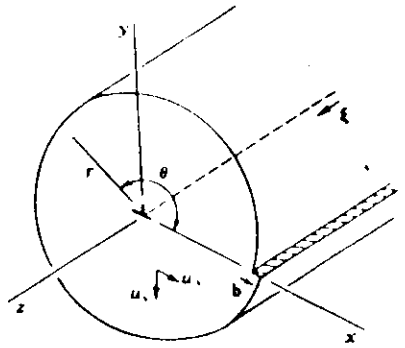
Burgess circuit:

$$b = \oint_{\Gamma} \frac{\partial u}{\partial l}\, dl$$



$$u_x = \frac{b}{2\Pi}\left[\operatorname{tg}^{-1}\frac{y}{x} + \frac{xy}{2(1-\nu)(x^2+y^2)}\right]$$

$$u_y = -\frac{b}{2\Pi}\left[\frac{1-2\nu}{4(1-\nu)}\ln(x^2+y^2) + \frac{x^2-y^2}{4(1-\nu)(x^2+y^2)}\right]$$



$$\sigma_{rr} = \sigma_{\theta\theta} = \frac{\mu b \sin\theta}{2\Pi(1-\nu)r}$$

$$\sigma_{r\theta} = \frac{\mu b \cos\theta}{2\Pi(1-\nu)r}$$

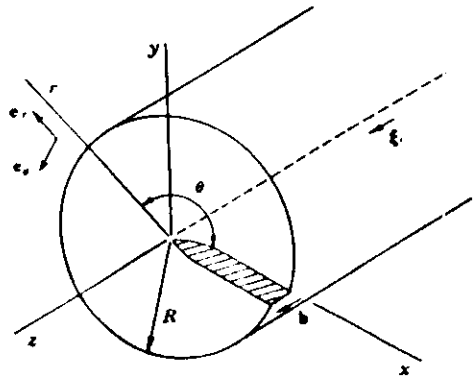
$$\sigma_{zz} = \nu(\sigma_{rr}+\sigma_{\theta\theta}) = -\frac{\mu b \nu \sin\theta}{\Pi(1-\nu)r}$$

$$\sigma_{rz} = \sigma_{\theta z} = 0$$

Strain energy / unit length

$$\frac{W}{L} = \frac{\mu b^2}{4\Pi(1-\nu)}\ln\frac{\alpha R}{b}$$

$$u_z(r,\theta) = b\frac{\theta}{2\Pi} = \frac{b}{2\Pi}\operatorname{tg}^{-1}\frac{y}{x}$$



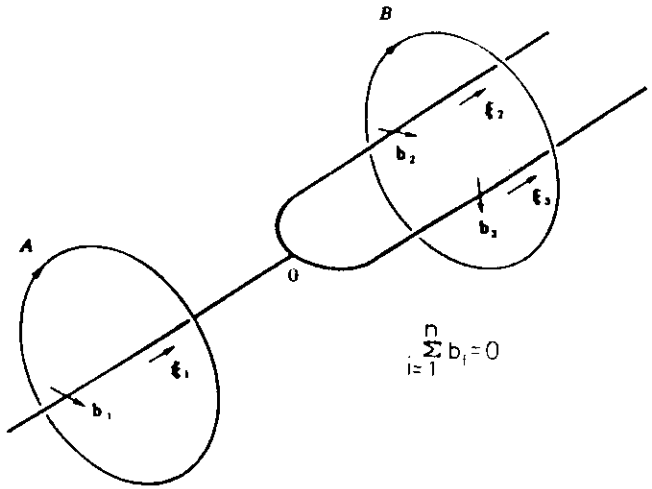
$$\sigma_{\theta z} = \frac{\mu b}{2\Pi r} \qquad \sigma_{zz} = \sigma_{r\theta} = \sigma_{rr} = \sigma_{\theta\theta} = \sigma_{rz} = 0$$

$$\mu = c_{44}$$

Strain energy / unit length (finite cylinder of radius R):

$$\frac{W}{L} = \int_{r_o}^{R}\frac{(\sigma_{\theta z})^2}{2\mu}\,2\Pi\,r\,dr = \frac{\mu b^2}{4\Pi}\ln\frac{R}{r_o}$$

7.5. EQUIVALENT BURGERS CIRCUITS



7.6. PARTIAL DISLOCATIONS

Frank dissociation circuits:

Crystal structure	Stable b	Marginal stability b
fcc	½⟨110⟩	⟨100⟩
bcc	½⟨111⟩,⟨100⟩	
hcp	⅓⟨11$\bar{2}$0⟩,⟨0001⟩	⅓⟨11$\bar{2}$3⟩
Diamong cubic	½⟨110⟩	⟨100⟩
NaCl	⟨110⟩	⟨200⟩

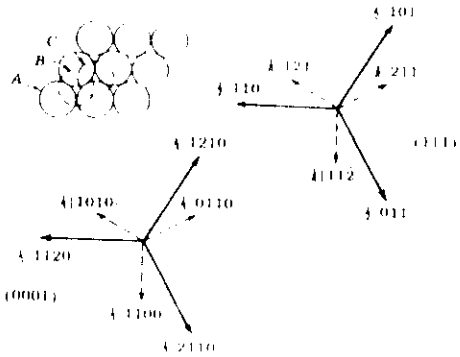
7.7. PLANAR FAULTS IN FCC METALS

Pure metals

Normal Packing:

fcc : --- A B C A B C --- {111} planes

hcp : --- A B A B A B --- {1000} planes



Projection normal to the (111) plane showing the three types of stacking positions A, B, and C. fcc and hcp vector notations are also presented

Twin in fcc : --- ABCABCBACBA ---

Stacking fault

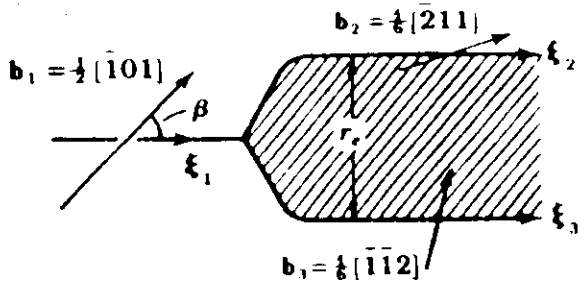
Intrinsic: --- ABCABC'BCABC ---

Extrinsic: --- ABCABCBABC ---

Higher energy faults (not considered feasible):

--- ABCABC'CABCABC ---

Shockley Partials



$$\frac{1}{2}\,[\bar{1}01] \;-\; \frac{1}{6}\,[\bar{2}11] \;+\; \frac{1}{6}\,[\bar{1}\bar{1}2]$$

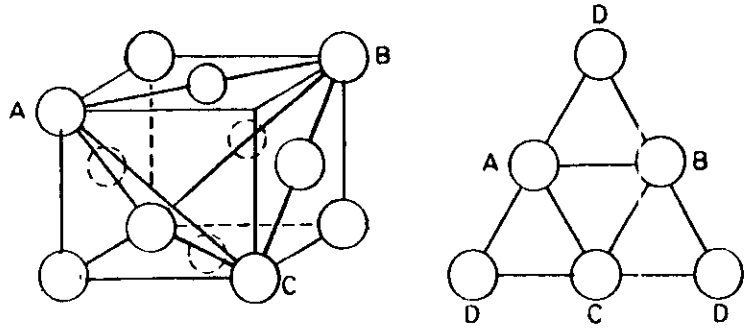
Energy equilibrium for two parallel Shockley partials at a distance r.

The formation of the fault between the partials increase the energy in $\gamma_I\, r$ per unit length. This is compensated by the gain in energy in separating the partial dislocations:

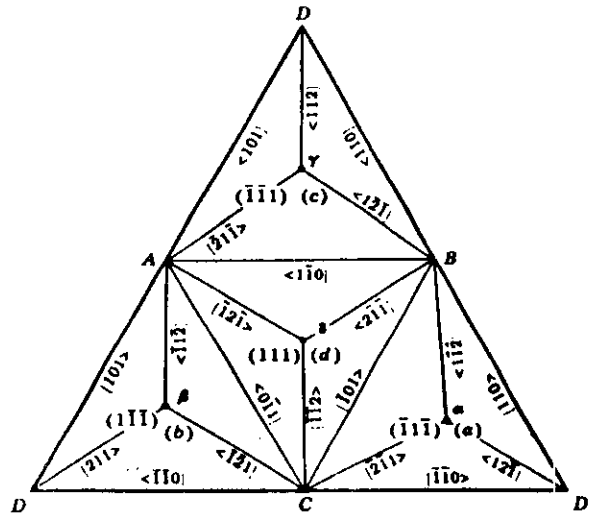
$$\gamma_I \;-\; \frac{\mu}{2\Pi\, r_e}\left[(\mathbf{b}_2\cdot\xi_2)\,(\mathbf{b}_3\cdot\xi_3) + \frac{(\mathbf{b}_2\wedge\xi_2)\cdot(\mathbf{b}_3\wedge\xi_3)}{(1-\nu)}\right]$$

where r_e is the equilibrium separation in an elastic isotropic medium.

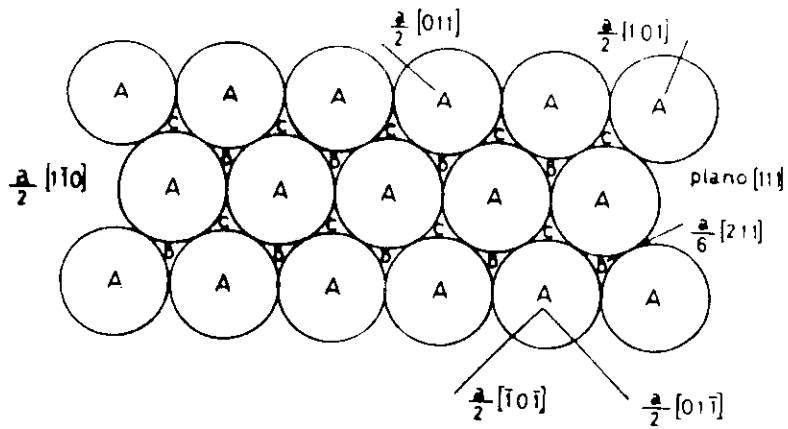
fcc metals



Thomson tetrahedron



fcc atomic stacking

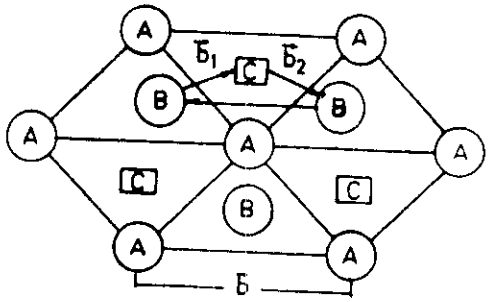


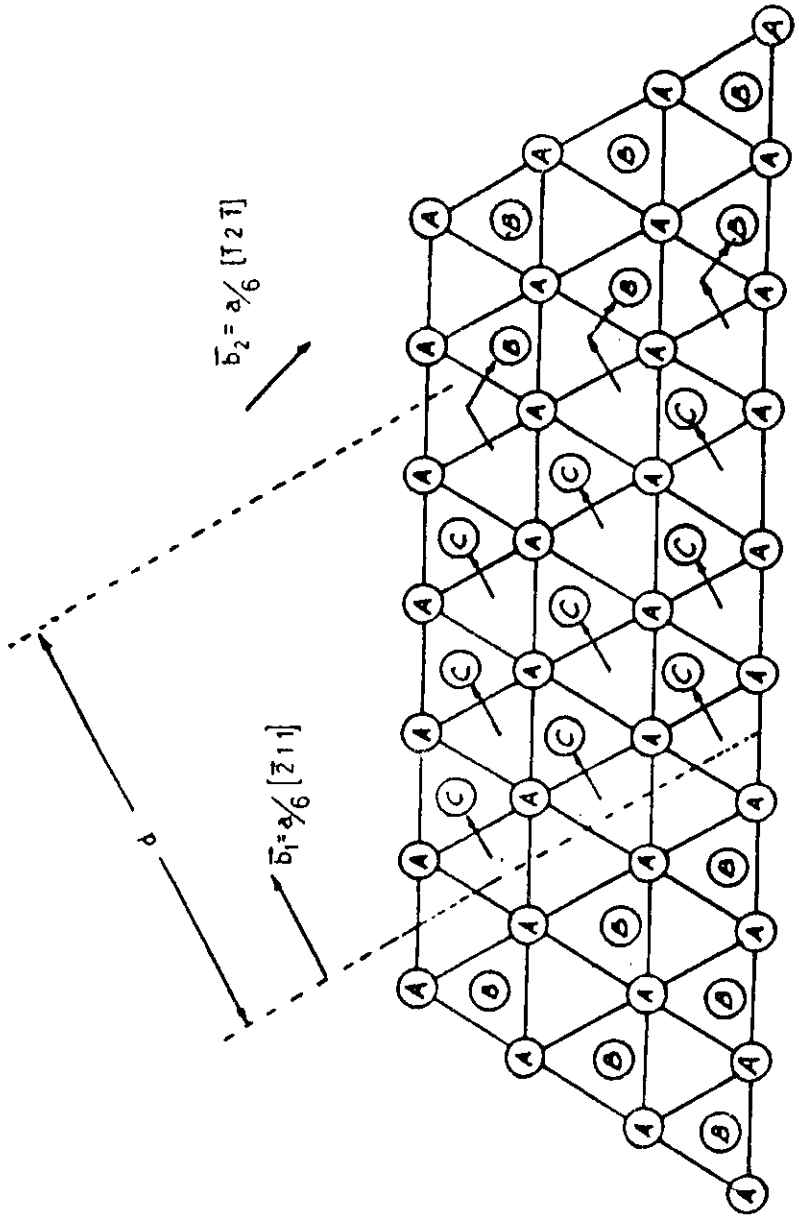
Possible dissociation:

$$a/2\ (1\bar{1}0) \rightarrow a/6\ (\bar{2}11) + a/6\ (\bar{1}2\bar{1})$$

Frank criteria:

$$b^2 = 1/2 > 1/6 + 1/6 = 1/3$$

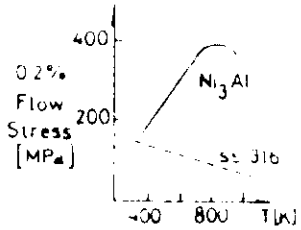




Continuum theory of dislocations success for its exploitation long range effects:

- mutual interaction of dislocations
- interaction with other defects, etc.

In general, plasticity of pure fcc metals.



However, it does not explain:

- flow stress dependence on crystal orientation and temperature of bcc metals
- Idem hcp
- annomalous yield behavior in $L1_2$ alloys (Ni_3Al, Ni_3Ge, Ni_3Co)

↓

DISLOCATION CORE EFFECTS / TECHNOLOGICAL RELEVANCE

Also relevant:

- Impurities segregation to surfaces, grain boundaries (Boron case).

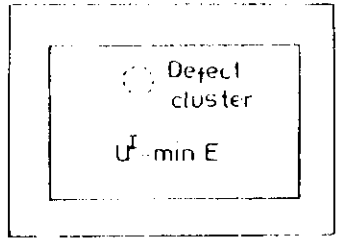
↓

IMPORTANT TO KNOW CONFIGURATION OF EXTENDED DEFECTS!!

↓

CALCULATION OF LATTICE DEFECTS STATICS AND DYNAMICS

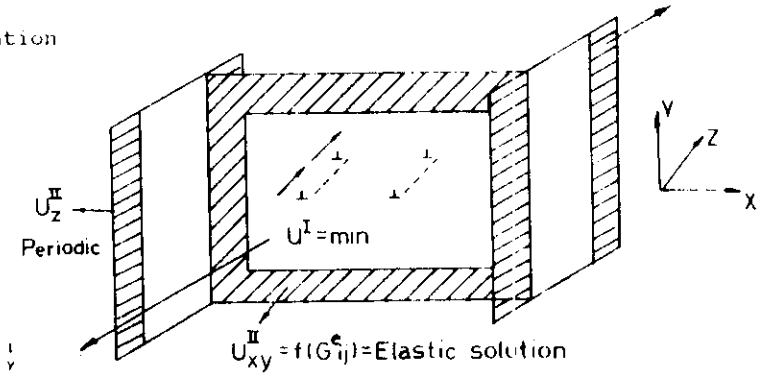
Point Defect or small cluster



$u_i^{II} = G_{ij,k}\ P_{jk}$

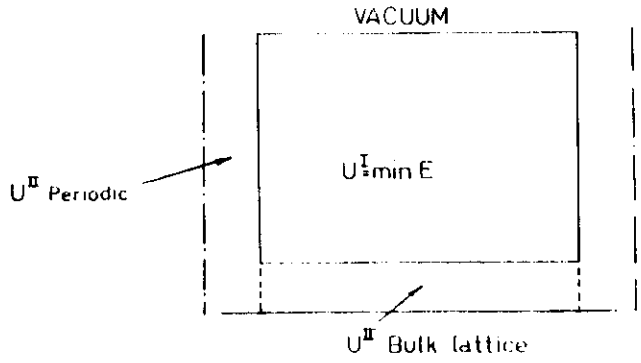
$P_{jk} = \sum_{(l,l')_j} \phi_{kj}(l,l')\ u_j^I(l')$

Dislocation



$U_z^{II} = U_z^I,\ U_{x\ y}^{I\ I}$

Free surface



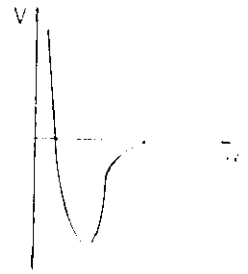
8.3. CALCULATION OF AN EXTENDED DEFECT CORE STRUCTURE

It may involve relaxing the atomic coordinates of [illegible] 45.000 atoms, i.e. 45.000 to 135.000 degrees of freedom.

Even now, first principle calculation is not possible.

NEED OF EMPIRICAL INTERATOMIC POTENTIALS

8.4. PAIR POTENTIALS



Ensamble N atoms:

$$E_{tot} = 1/2 \sum V(R_{ij})$$

Equilibrium:

$$\partial E_{tot} / \partial \Omega \; (\Omega = \Omega_{eq}) = 0$$

"Cauchy relation": $C_{12} = C_{44}$

8.5. CONSTANT VOLUME POTENTIALS

$$E_{tot} = 1/2 \sum V(R_{ij}) + U(\rho)$$

U: part of the energy which depends on average density ρ.

Equilibrium is attained at P (actually, volume) = ρ_c

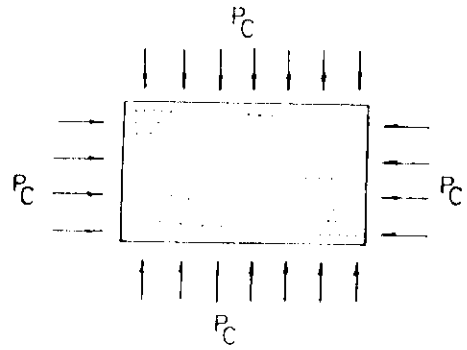
ρ_c = constant

$$\Downarrow$$

$$C_{12} \neq C_{44}$$

but a "Cauchy" pressure must be applied to keep the volume from expanding/contracting.

$P_c = C_{12} - C_{44}$



Interatomic potentials either completely empirical or pseudo-potential based.

Success in predicting:

- Possible point defects configuration
- Dislocation structure in fcc and bcc
- Structural trends on ordering, stacking faults, etc.

8.6. ENGLERT, TOMPA AND BULLOUGH'S PAIR POTENTIAL

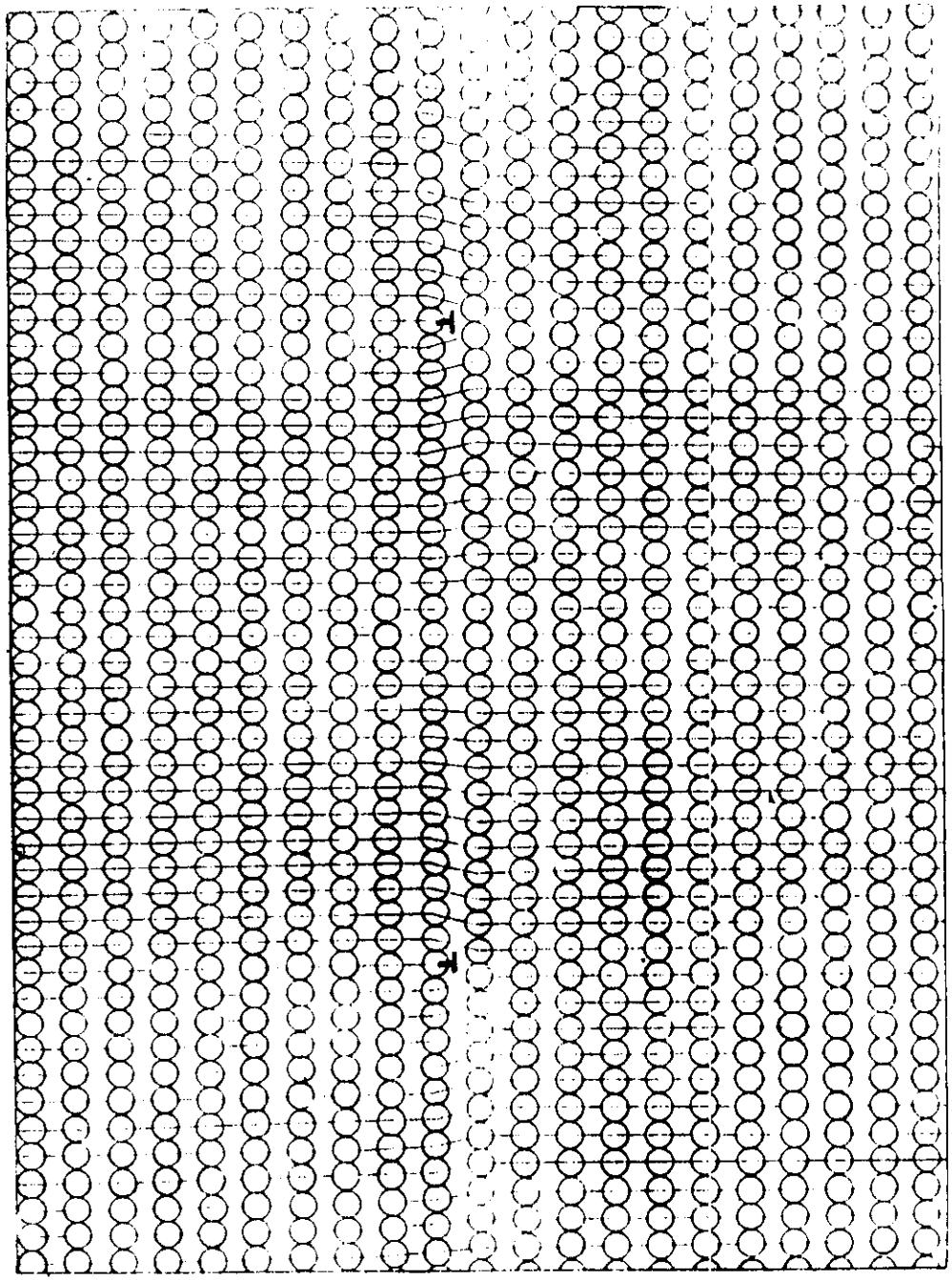
1) Distance less than first neighbour: radiation damage data.

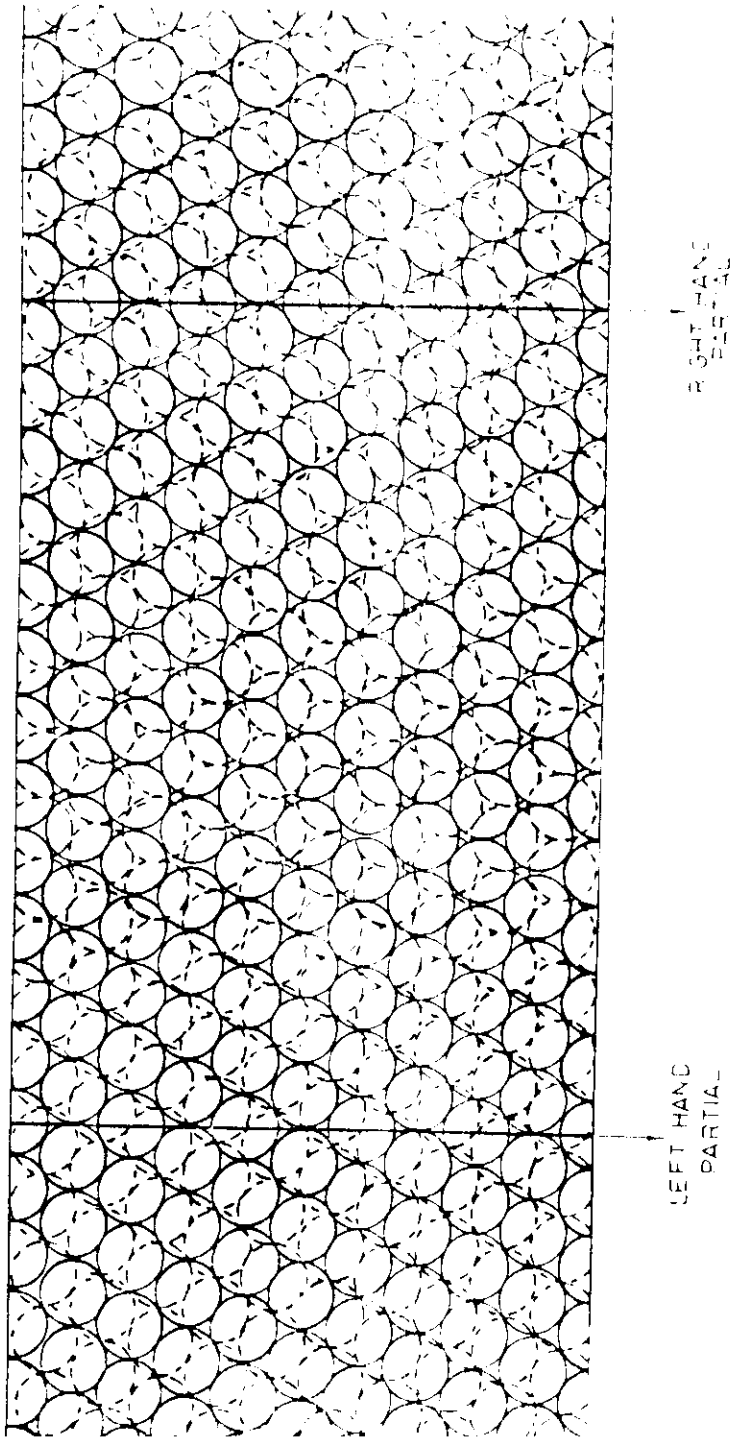
2) Adding volume constraints holds the atoms in stable fcc lattice (a_o = 3.608 Å).

3) $dV / dr |_{r1,r2}$, $d^2V / dr^2 |_{r1,r2}$: fit elastic constants and phonon dispersion data.

4) E_f = 1.14 eV

5) γ = 70. ergs/cm^2





2.2 SIMULATION OF ELECTRON MICROSCOPIC INTENSITY PROFILES IN THE COLUMN APPROXIMATION

$$d\Phi / dz = 2\pi i (A + (\beta_g)_{diag}) \Phi$$

Φ: amplitudes of electron waves

Defect structure enters in the matrix:

$$\beta_g = d (g \cdot R(z)) / dz$$

In the experimental condition for edge dislocation imaging:

$g \cdot b = 2$ $g = [\bar{2}20]$, systematic row: [220], [660] set at Bragg condition

Relevant distortion:

$$\beta_{xz} = \partial R_x (z) / \partial z \qquad x = [110]$$
$$z = [111]$$

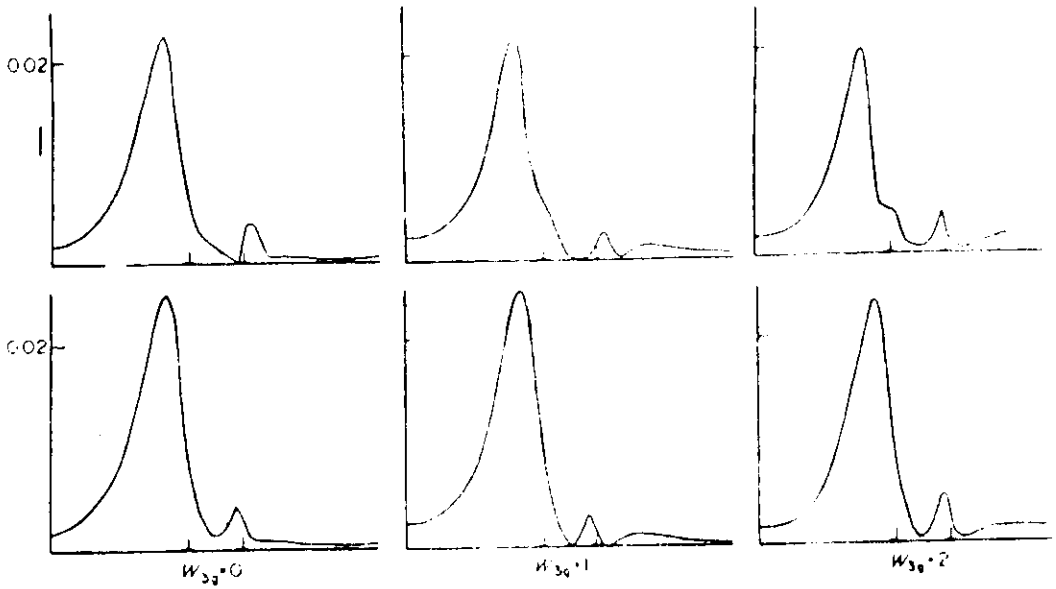


Fig. 2. Intensity profiles of $\mathbf{g}.\mathbf{b} = 2$ weak-beam images of the dissociated edge dislocation in copper for $w_{3g} = 0, 1, 2$. The top row has been calculated from the atomic model and the bottom row from elasticity for the same partial separation of 3·2 nm.

Table 1

γ_{SF} (erg cm^{-2})	Model	Partial separation (nm)	Model	Peak separation (nm)
78	Atomic	3·2	Atomic	5·4 ± 0·4
70	Atomic	3·2	Elastic	4·3
70	Elastic	2·0	Elastic	3·5
41*	Elastic	5·8*	Elastic	4·7 ± 0·6*

* Stobbs & Sworn (1971).

8.8. DRAWBACKS OF CONSTANT VOLUME POTENTIALS (APART FROM NEED OF CAUCHY PRESSURE)

1) Quantitative ones:

- $E_f^v = E_c$ $\quad E_f^v$: vacancy formation energy

E_c : cohesive energy

- Wrong prediction of T_m

2) Qualitative ones:

- As generally $P_c > 0$ → First layer at a free surface relaxes outwards (contrary to most experimental findings).

- No surface reconstruction is predicted.

8.9. FORMATION ENERGY OF DEFECTS

Formation energy of the vacancy (cohesive energy)

$$E_c = -(n/2)\,\Phi(d) + E_R^s$$

$$E_v = -(n/2)\,\Phi(d) + E_R^v$$

Where:

Φ = interaction pair potential

E_R^s = relaxation energy of the surface

E_R^v = vacancy elastic relaxation

This implies: $E_c = E_v$ within 20%

However (experimentally):

E_v / E_c:		
	Neon	1.05
	Ar	.95
	Kr	.66
	Al	.23
	Pb	.24
	Ni	.31
	Pt	.26
	Cu	.33
	Ag	.36
	Au	.25

8.10. EMBEDDED ATOM, GLUE, FINNIS AND SINCLAIR, EMPIRICAL MANY BODY INTERATOMIC POTENTIALS

$$E_{tot} = 1/2 \sum V_{ij}(R_{ij}) + \sum f_i(\rho_i)$$

local density: $\rho_i = \sum_{i \neq j} \phi_i(R_{ij})$

total e^- density at atom i associated with the host lattice effective medium

f_i is the energy to embed an atom into this e^- density.

Success into predicting:

Pure metals: Defect structure
Surface structure and reconstruction
Mechanical properties: fracture, effect of impurities

Alloys: Phase stability
Segregation
Surface structure *
Dislocation structure *

* We shall show some results hereafter.

Embedded Atom

$$E_{tot} = 1/2 \sum_{i,i\neq j} V_{ij}(R_{ij}) + \sum_i f_i(\rho_i)$$

(Pair Inter.) (N Body term)

$\rho_i = \sum_{j\neq i} \phi_i(R_{ij})$ (Density of atom i)

R_{ij} = distance from i to j

Daw and Baskes:

Impurity in host (up to cohesion) "umperturbed host potential is determined by electron density..." "...energy of host with impurity is a functional of host and impurity potentials".

"Energy of host with impurity is a functional of the umperturbed host electron density and a function of the impurity type and position":

$$E = F_{z,\phi}[\rho_h(r)]$$

Impurity problem identical to an impurity in jellium.

Ansatz: $E_{tot} = \sum_i F_i(\rho_{h,i})$

where

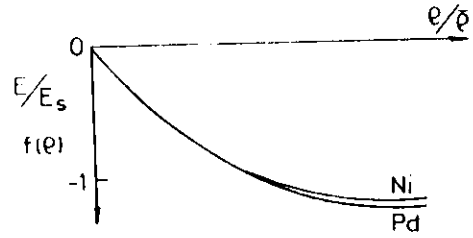
F_i: embedding energy **F vs F**

More physical basis:

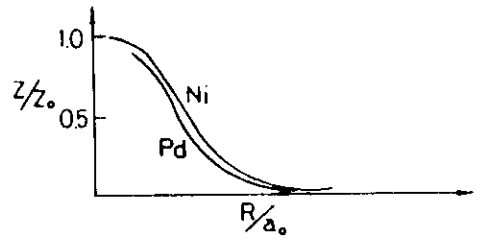
- J. Harris; Phys. Rev. B 31 (1985) solves overlapping of atoms i by $\rho_i = \rho^{self\ consistent}$

- Jacobsen et al., Phys. Rev. B 35, 7423 (1987), First principle approach (needs, however, fitting of e⁻ function).

Daw and Baskes:



Es: Sublimation energy



$V_{ij} = [z_i(r)\ z_j(r)] / r$

$\phi(-)$ [$\rho(r)$]: Clementi et al., Atomic Data and Nuclear Data Tables 14, 3 and 4, calculations for atomic electron density.

Finnis and Sinclair:

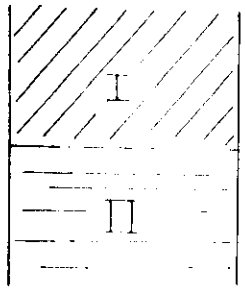
$$\phi(r) = (r-d)^2 \quad r \leq d$$
$$0 \quad r > d$$
$$V(r) = (r-c)^2(c_0 + c_1 r \quad c_2 r^2) \quad r \leq c$$
$$0 \quad r > c$$
$$f(\rho) = -\rho^{1/2}$$

9. FREE SURFACE CONFIGURATION

The largest and certainly most important of the defects in the solid is its free surface. This connects the body with its environment and either it is important in itself into determining the behavior of the solid (for example, the ratio: surface/volume determines the chemical activity and efficiency in catalytic processes) or as a path to modify the body properties during its processing or performance (for example, gas absorption, embrittlement, corrosion, etc. etc.); also, it is the main initiation place for phase transformation. Several physical and chemical aspects of the surface are relevant to phase nucleation, growth and segregation in the bulk of the solid. However, for consistency, in this lecture we shall concentrate on the lattice statics of the free surface.

The study of the lattice static configuration has received a renewed attention lately when empirical interatomic potentials based on the Embedded Atom Method have become available.

9.1. INTERPHASE ENERGY



$$V(\vec{X}) = \sum_{\alpha\beta} \left[V(\vec{X}_{\alpha\beta})_{\beta\in I} + V(\vec{X}_{\alpha\beta})_{\beta\in II} \right]_{\alpha\in I,II}$$

Rigid displacement:

$$X_{\alpha\beta} = x_{\alpha\beta} + \Delta X \qquad if\ \alpha\in I, \beta\in II$$

$$\Delta X : \quad \frac{\partial V(x)}{\partial x} = 0 \quad \rightarrow$$

$$\lim_{\Delta x\to 0} \frac{\left[V_{\substack{\alpha\in I \\ \beta\in II}} (X_{\alpha\beta} + \Delta x) - V_{\substack{\alpha\in I \\ \beta\in II}} (X_{\alpha\beta}) \right]}{\Delta X} = 0$$

$\vec{x}$: 3 n dimension vector of atomic position at perfect lattice (+ rigid)

$\vec{\mu}$: 3 n dimension vector of atomic displacements (without rigid body displacement)

$$V(\vec{x} + \vec{\mu}) - V(\vec{x}) = - \sum_{lx} F_i^{I,II}(lx) \cdot [\mu_i^{II}(lx) - \mu_i^{I}(lx)] + \frac{1}{2} \sum_{lx,l'x'} \varphi_{ij}^{*}(lx, l'x') \mu_i^{I,II}(lx) \mu_j^{I,II}(l'x') + \ldots$$

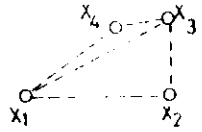
$$\underline{\Phi}^{*} = \underline{\Phi} + \underline{\xi}$$

$\underline{\Phi}$: perfect lattice force constant
$\underline{\xi}$: defect force constant

i.e.: Free surface or interphase

$$\underline{\xi}(l_I x_I, l'_{II} x'_{II}) = - \varphi(l_I x_I, l'_I x'_I) + \xi^{*}(l_I x_I, l'_{II} x'_I)$$

$(l_I x_I, l'_{II} x'_{II}) = 0$ at free surface



If

$$F(lx) = F^{0}(l) + \Delta F(lx)$$

$$\mu(lx) = \mu^{0}(l) + \Delta\mu(lx)$$

$$F^{0}(l) = \sum_{x} \frac{F(lx)}{N_x}$$

$$\mu^{0}(l) = \sum_{x} \frac{\mu(lx)}{N_x}$$

System of equations:

$$N_x F_i^{0} = \Phi_{ij}^{ll'}(l,l') \mu_j^{0}(l') + \Phi_{ij}^{lx}(l,l'x') \Delta\mu_j(l'x')$$

$$\Delta F_i(lx) = \Phi_{ij}^{xx'}(lx,l'x') \Delta\mu_j(l'x') + \Phi_{ij}^{lx}(lx,l') \mu_j^{0}(l')$$

$$\Phi_{ij}^{ll'}(l,l') = \sum_{xx'} \varphi_{ij}^{*}(lx,l'x')$$

$$\Phi_{ij}^{lx}(l,l'x') = \Phi_{ij}^{lx}(l'x',l) - \sum_{x} \varphi_{ij}^{*}(lx,l'x')$$

$$\Phi_{ij}^{xx}(lx,l'x') = \varphi_{ij}^{*}(lx,l'x')$$

Can be solved by Green function approach.

Concept of static "acoustic" and "optic" distortion.

Concept of dispersive medium:

Elastic constants ($\Delta F = 0$) →

$\Delta\underline{\mu} = \underline{G}^{xx'} \underline{\Phi}^{lx} \underline{\mu}$ $\quad \underline{G}^{xx'} = (\underline{\Phi}^{xx'})^{-1}$

$\underline{\mu}^{0} = \underline{G}^{ll'} \underline{T}^{ll'} (N_x \underline{F}^{0})$ $\quad \underline{G}^{ll'} = (\underline{\Phi}^{ll'})^{-1}$

( ):lattice response

$$T_{ij}^{ll'} = [I_{ij}^{ll'} - \Phi_{ik}^{lx}(l,l^{II}x^{II}) G_{k\mu}^{xx'}(l^{II}x^{II}, l^{III}x^{III}) \Phi_{\mu j}^{lx}(l^{III}x^{III}, l')]^{-1}$$

Rippling is just one kind of antisymmetric distortion.

We shall now summarize some computer simulation results for free surfaces.

In general, one should expect either a contraction or expansion of the first atom layers which monotonously decay towards the bulk.

However, the result is a:

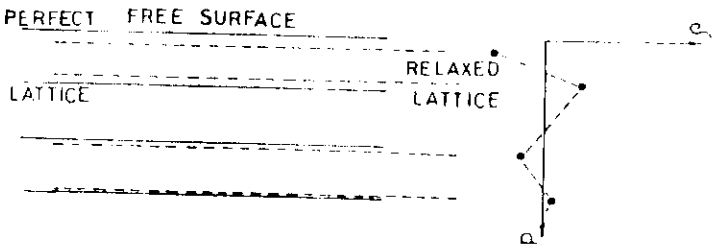
contraction or expansion at the free surface

+

oscillatory relaxation perpendicular to this surface.

Actually, the latter is a lattice effect.

It was predicted in the early seventies by G. Allan and M. Lannoo (Surf. Sc. 40, 375 (1973); Phys. Stat. Sol. (b) 74, 409 (1976)) based on a model which explicitly takes into account the non-local effects in an harmonic expansion of the lattice energy.



This model includes two quadratic terms in the energy expansion as a function of the interphase separations, one of them being proportional to the product of neighbour interplanar distances ($\alpha\, d_{n,n+1}\, d_{n+1,n+2}$) and a second quadratic in those distances $\beta (d_{n,n+1})^2$, where α, $\beta > 0$.

This effect was "rediscovered" by U. Landman, R.N. Hill and M. Mostoller, Phys. Rev. 21, 448 (1980) and has received quite a large atention more recently.

If free surfaces are modelled by computer simulation and using pair interatomic potentials, not only quantitative wrong results may be obtained but no oscillation may be predicted. In pure metals oscillations in the perpendicular displacements are due to an equilibrium between the pair interaction terms and the many body ones. A contraction/expansion of the surface atoms implies a change in the local density of inner atoms, which in turn must be compensated by the opposite displacement (expansion / contraction) of more inner layers. This results in an intrinsically oscillatory static relaxation.

For alloys, an extra effect of "rippling" due to the difference in cohesive energy for different elements of the alloy appears. This is summarized by Savino and Farkas, Phil. Mag. 58, 227 (1988). Some parts of that work will be summarized here.

Let us first summarize previous theoretical and experimental results for the NiAl system.

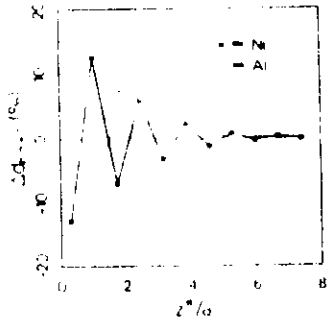
Experiments:

* NiAl (110) surface · rippling (Al out, Ni in)
  first layer inwards relaxation
  H.L. Davis, J.R. Noonan, Phys. Rev. Lett 54, 566 (1985)

* Ni_3Al (100) surface · mixed composition termination; Al out
  Sondericker et al., Solid St. Comm. 31, 175 (1985), Phys. Rev. B 33, 900 (1986)

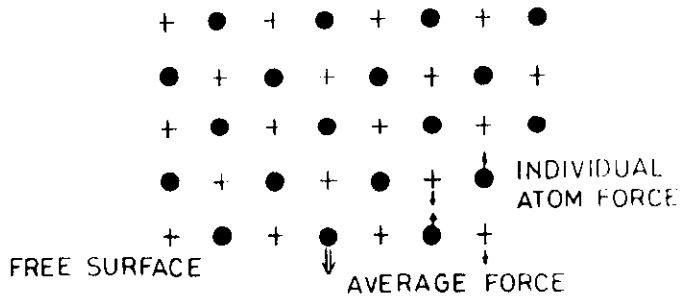
Theory:

* (111), (110) surface · Al out
  S.M. Foiles, M.S. Daw, J. Mater. Res. 2 (1), 5 (1987)
  Chen et al., MRS Boston Meeting (1986), Phys. Rev. Lett 57, 1308 (1986)



E_{coh} Al < (model) < E_{coh} NiAl < E_{coh} Ni < (exp) < E_{coh} Ni_3Al

Rippling: Equilibrium between body, "local volume", forces and pair ones.

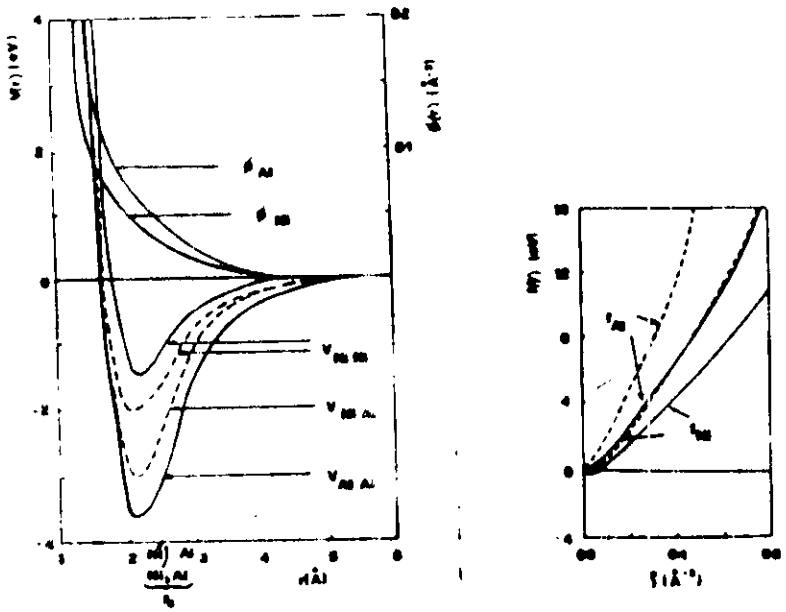


9.3. EAM INTERATOMIC FORCES IN Ni_3Al

$$E_{tot} = \frac{1}{2} \sum_{i,j=1}^{N} V_{ij}(R_{ij}) + \sum_i F_i(\rho_i)$$

$$\rho_i = \sum_{j=1} \phi_j(R_{ij})$$

The Embedded Atom Interatomic Potential was calculated by A.F. Voter and S.P. Chen, Mat. Res. Soc. Proc., Boston 82, 175 (1987):



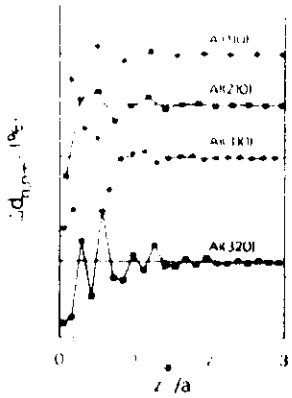
Interatomic potential functions for Ni, Al and Ni/Al alloys, Voter *et al* (1987). Full and dotted lines correspond to a set of energy functions related among themselves by the relations discussed in the text.

TABLE I. Metal properties used in fit. Calculated values of a_0, E_{coh} and B match experiment exactly due to the way F($\bar{\rho}$) is determined. Superscripts are the experimental references (a=Ref. 14, b=Ref. 15, c=Ref. 16, d=Ref. 17, e=Ref. 18, f=Ref. 19, g=ref. 20, h=Ref. 21).

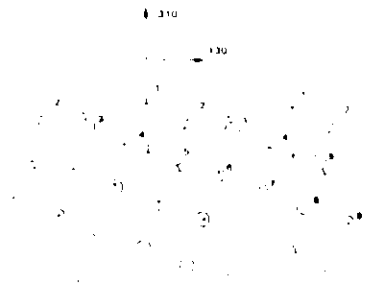
Property	Ni		Al	
	expt.	calc.	expt.	calc.
a_0(Å)	3.52[a]		4.05[a]	
E_{coh}(eV)	4.45[b]		3.36[c]	
B (10^{12}erg/cm^3)	1.81[d]		0.79[d]	
C_{11}(10^{12}erg/cm^3)	2.47[d]	2.44	1.14[d]	1.07
C_{12}(10^{12}erg/cm^3)	1.47[d]	1.49	0.619[d]	0.652
C_{44}(10^{12}erg/cm^3)	1.25[d]	1.26	0.316[d]	0.322
ΔE^f_{1v} (eV)	1.60[e]	1.60	0.75[f]	0.73
D_e (eV)	1.95[g]	1.94	1.60[h]	1.54
R_e (Å)	2.29	2.23	2.47[h]	2.45
χ (rms%)	0.75		3.85	

TABLE II. Metal properties used to fit the Ni_3Al cross potential. Superscripts are the experimental references (a=Ref. 22, b=Ref. 23, c=Ref. 24, d=Ref. 25, e=Ref. 26, f=Ref. 14).

Ni_3Al properties	expt.	calc.
a_0(Å)	3.567[a]	3.573
E_{coh}(eV)	4.57[b]	4.59
C_{11}(10^{12}erg/cm^3)	2.30[c]	2.46
C_{12}(10^{12}erg/cm^3)	1.50[c]	1.37
C_{44}(10^{12}erg/cm^3)	1.31[c]	1.23
ΔE^f_{1v} (eV)	1.6±0.2[d]	1.64(Ni), 1.87(Al)
SISF(111) (mJ/m^2)	10±5[e]	13
APB(100) (mJ/m^2)	140±14[e]	83
APB(111) (mJ/m^2)	180±30[e]	142
B2 NiAl properties		
a_0(Å)	2.88[f]	2.87
E_{coh}(eV)	4.51[b]	4.38



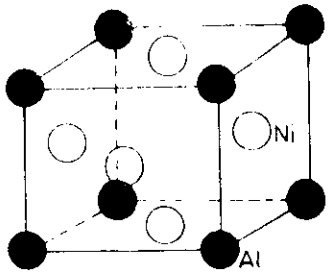
Surface relaxations of the pure Al (110), (210), (310) and (320) surfaces as functions of depth. The depth z is measured in units of $\frac{1}{2}\sqrt{2}a$, where a is the lattice constant and $z=0$ is the midpoint between the atoms on layer n and $n+1$. Each tick mark on the vertical axis corresponds to 10%.



Relaxation of the Al (310) surface. The circles represent unrelaxed (truncated bulk) atomic positions (dotted atoms lie in a plane $\frac{1}{2}a$ below the other atoms). The vectors show the relaxation motions of the atoms, magnified 10 times.

Ref.: S.P. Chen, A.F. Voter, D.J. Srolovitz

5.4. Ni_3Al AND Ni_3Al RESULTS



Free surfaces studied:

(100) , (110) , (120) , (111)

in papers included in "Additional Lecture Notes".

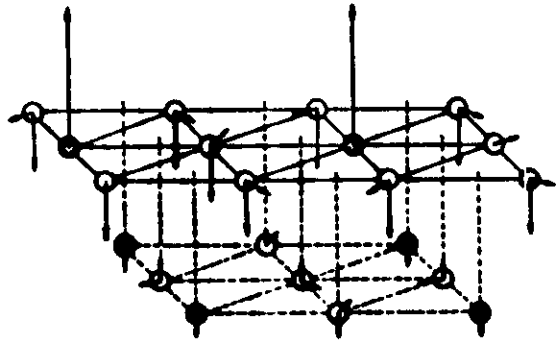
"Acoustic" body forces, perpendicular to (111) surface contract first interlayer distance.

"Optical" forces → - Rippling, Al outwards
- Oscillations parallel to free surface

"Optical" forces:

While forces mainly concentrated onto second layer, displacements parallel to the surface appear also in first layer.

Also, as in Ni atoms in first layer move inwards, those in second layer also do so, trying to compensate change in local density.



Atomic displacements of the first two layers of a (111) surface in Ni_3Al. The arrows showing the displacement are in units of lattice distance multiplied by 50.

9.5. SURFACE RESTRUCTURING

Due to relaxation, surface configuration relaxes outwards from bulk lattice on.

Several authors have treated this problem, for example: A. Bartolini, F. Ercolessi and E. Tosatti, "The Structure of Surfaces II", ed. J.F. Van der Veen and M.A. Von Hove (Berlin, Springer Verlag), 132 (1988).