INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
34100 TRIESTE (ITALY) - P.O.B. 586 - MIRAMARE - STRADA COSTIERA 11 - TELEPHONE: 2240-1
CABLE: CENTRATOM - TELEX 460392 - I

SMR/388 - 42

SPRING COLLEGE IN MATERIALS SCIENCE
ON
'CERAMICS AND COMPOSITE MATERIALS'
(17 April - 26 May 1989)

SIMULATION OF PERFORMANCE OF NON-HOMOGENEOUS MATERIALS
(Lecture III)

E.J. SAVINO
Comision Nacional de Energia Atomica
Departamento de Materiales
Avda del Libertador 8250
Ra-1429
Buenos Aires
Argentina

Taylor - Bishop and Hill (1951)

1- Compatibility (Taylor approach)

At each grain $d\underline{\underline{\varepsilon}}^g = d\underline{\underline{\varepsilon}}^o$

2- At each grain g :

There are 5 systems s ; where:

$$m_{ij}^{(s)} \sigma_{ij} = \tau_c^{(s)}$$

For all other systems :

$$m_{ij}^{(s)} \sigma_{ij} \leq \tau^{(s)}$$

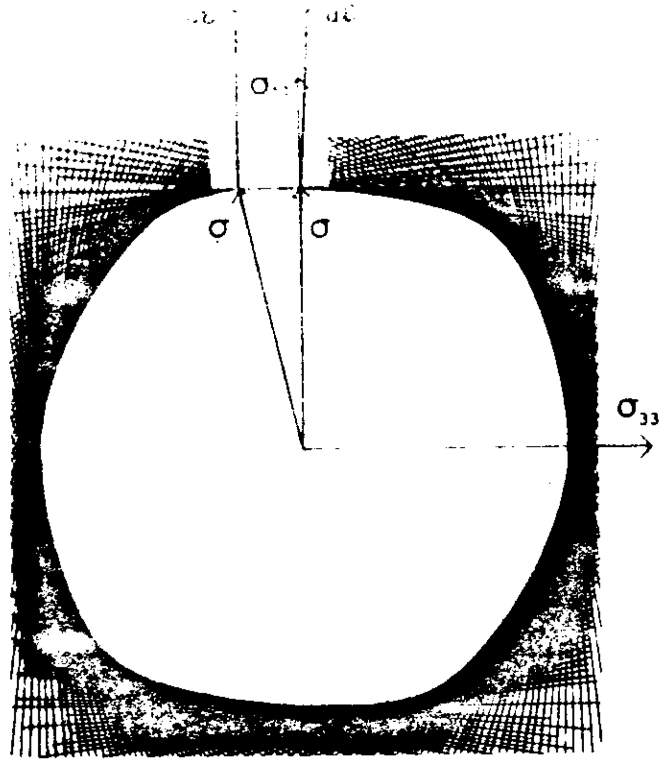
Those equations determine a closed surface in the space of possible $\underline{\underline{\sigma}}$ (5 dimensions) ;

<u>Yield</u> <u>loci</u> :

$$m_{ij} := \frac{1}{2|b|}\left(b_i n_j + b_j n_i\right)$$

$$dw = \sigma_{ij}\, d\varepsilon^{\circ}_{ij} = \tau_c^{(s)}\, d\gamma^{(s)} \rightarrow \min$$

$$\sum_{s=1}^{S} m_k^{(s)}\, d\gamma^{(s)} = d\varepsilon_k^{\circ}$$



(a)

Fig. 11. (a) A polycrystal yield surface derived by computer simulation, after torsion to $\gamma_0 = 1$, with fixed ends. Continued shear with fixed ends demands a compressive stress (at the apex to the left); continued shear with free ends would give the length change corresponding to the inclination of the normal at the top.

How does one find the shear at each system (s) ?

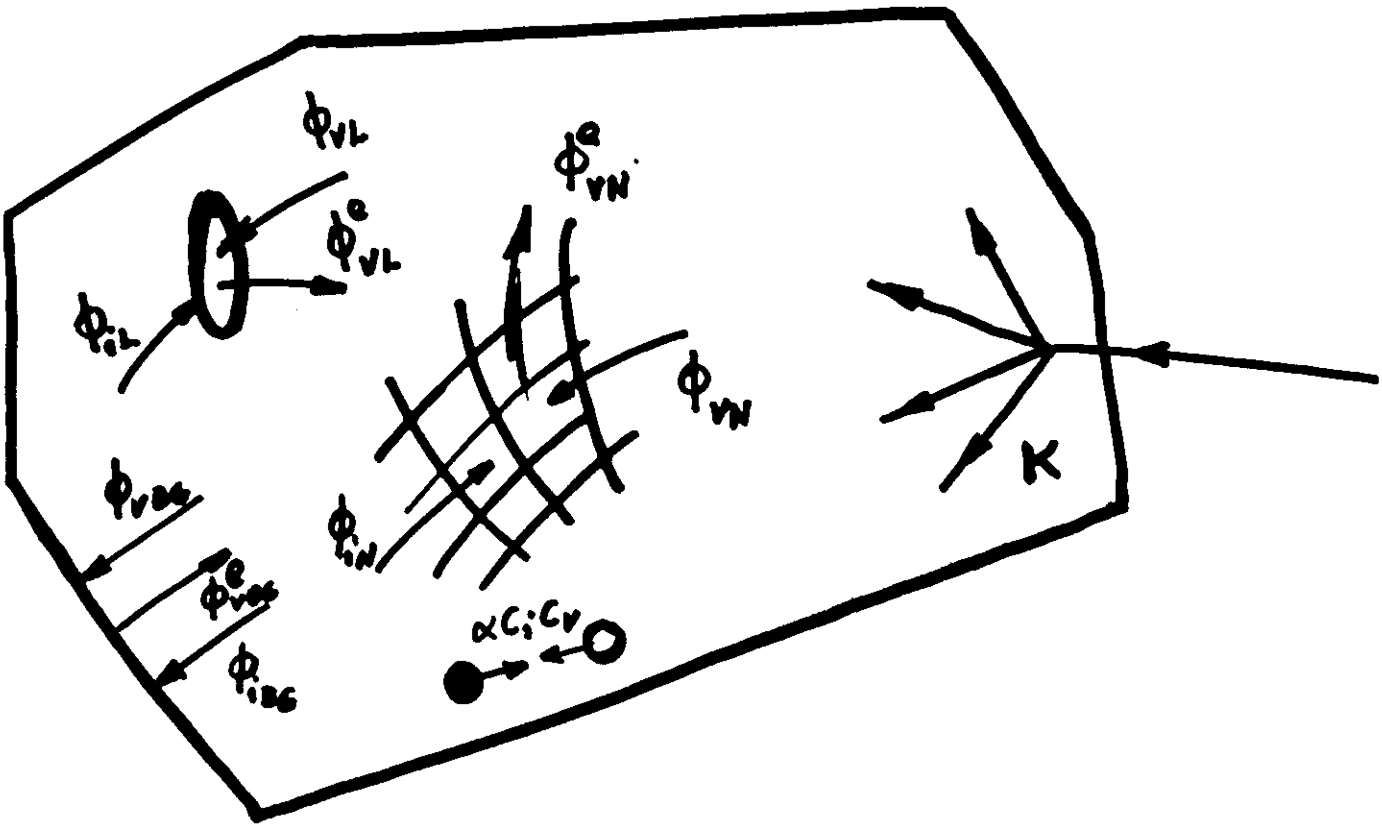
For the same 5 systems s

$$\sum_{s=1}^{5} m_{ij}^{(s)} \, d\gamma^{s} = d\varepsilon_{ij}^{p} = d\varepsilon_{ij}^{\circ}$$

Such that

$$dw = \sum_{s=1}^{5} \tau_c^{(s)} \, d\gamma^{(s)} = \text{minimum}$$

with $\tau_c^{(s)} d\gamma^{(s)} \geq 0$



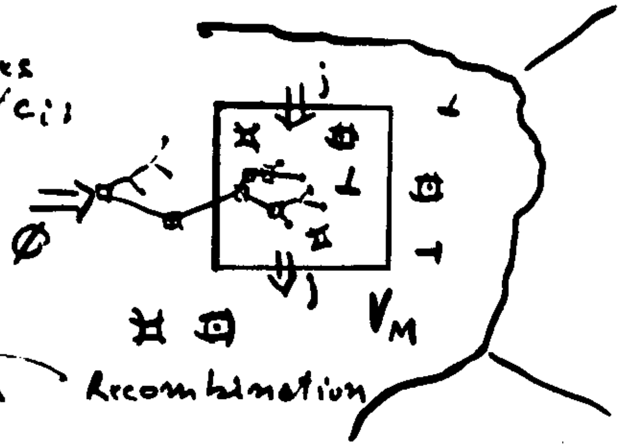
$$\frac{dC_i}{dt} = K - \phi_{is} + \phi^e_{is} - \alpha C_i C_v$$

$$\frac{dC_v}{dt} = K - \phi_{vs} + \phi^e_{vs} - \alpha C_i C_v$$

Finally

Rate theory (Brailsford, Bullough)

continuity equation for vacancies and interstitial concentration c_v / c_i



$$\partial c_v / \partial t + \underline{\nabla} \cdot \underline{j}_v = K - \alpha c_i c_v$$

$$\partial c_i / \partial t + \underline{\nabla}\, \underline{j}_i = K - \alpha c_i c_v$$

Defect production Recombination

Plus di, tri ... { vacancies, interstitials (we shall ignore for simplicity)

Effective medium (lossy)

Embedding procedure:

Assumptions { Periodic array of sinks; Random array

Rate equations: sink strength, emission term

$$\frac{d\langle c_v\rangle}{dt} + \sum_L \left(D_v k^2_{Lv} \langle c_v \rangle - K^e_{Lv} \right) - K - \alpha \langle c_i \rangle \langle c_v \rangle = 0$$

$$\frac{d\langle c_i\rangle}{dt} + \sum_L \left(D_i k^2_{Li} \langle c_i \rangle - K^e_{Li} \right) - K - \alpha \langle c_i \rangle \langle c_v \rangle = 0$$

Summary :

We have covered in the 3 lectures:

1 - All materials are inhomogeneous

2. However, when the engineer or the designer of a component looks at it, it behaves as a continuum !

3. How to relate the inhomogeneous microstructure, with a continuum ?
How to model the continuum ?
To answer those questions, we :
3.1 Reviewed continuum mechanics
3.2 Showed the need for realistic constitutive equations
3.3 Introduced the concept of effective medium

4. As examples we studied :
4.1 An effective elastic medium
4.2 Plasticity of textured (anisotropic) polycrystals.
4.3 Equations of lossy medium.

Guide to the use of the background material as illustration to the lectures:

Sarce - Savino : By using thermodynamics it finds a relation between macro and microvariables in an effective medium under stress and an irradiation flux.

Savino - Tomé : An application of the concept of lossy effective medium for explaining the large rate of creep found under irradiation.

2 papers by
Harriague - Savino : Show a parametric study of the influence of the models used for describ the thermal-mechanical performance into the calculation of parameters with stro technological relevance.

Savino - Harriague : shows that rate theory modelling can be used together and consistently with continuum mechanics calculations.