Forces on Dislocations

Plastic Deformation in Crystalline Materials

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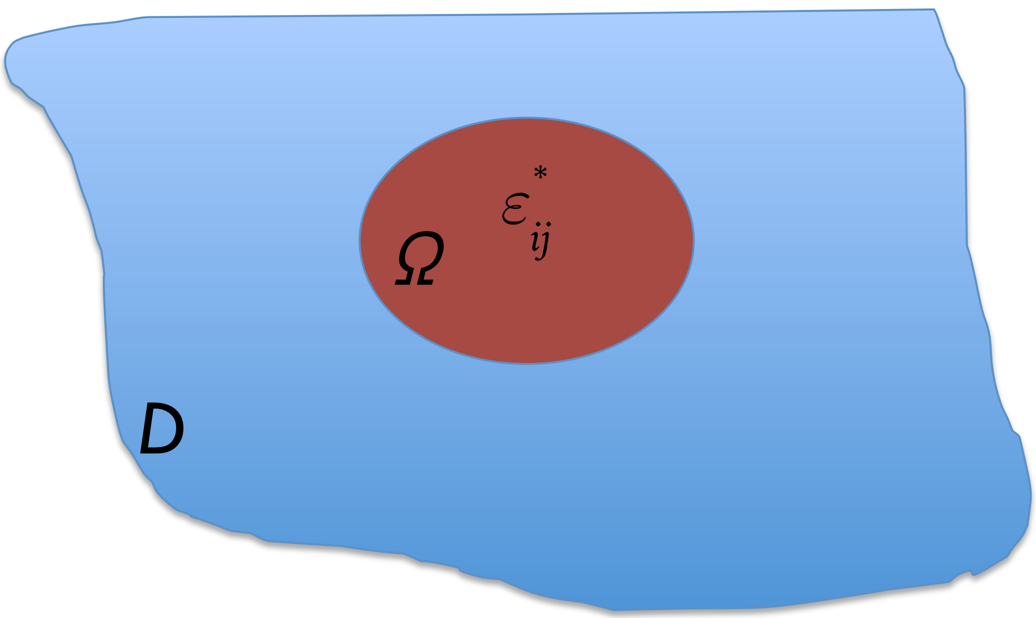
Lecture 9

Lemma: Energy of Inclusions

- Consider a finite body D, containing inclusions Ω. Material is either isotropic or anisotropic. Assume that eigenstrain ε^*_{ij} (inelastic strains such as plastic or thermal strains) is prescribed in Ω.



Lemma: Energy of Inclusions

- First let *D* be free of any external forces and surface constraints. The elastic strain energy is:

$$E_{el} = \frac{1}{2}\int_D \sigma_{ij}\varepsilon_{ij}^{(e)}\, dV$$

- Remember that $\varepsilon_{ij}^{(e)} = \varepsilon_{ij} - \varepsilon_{ij}^{*}$ and $\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$

- Integration by parts reveal that:

$$\int_D \sigma_{ij} u_{i,j}\, \mathrm{d}V = \int_S \underbrace{\sigma_{ij} u_i n_j}_{\sigma_{ij} n_j = T_i = 0}\, \mathrm{d}S - \int_D \underbrace{\sigma_{ij,j}}_{=0} u_i\, \mathrm{d}V = 0$$

- Therefore:

$$E_{el} = \frac{1}{2}\int_D \sigma_{ij}\varepsilon_{ij}^{(e)}\, dV = -\frac{1}{2}\int_\Omega \sigma_{ij}\varepsilon_{ij}^{*}\, dV$$

Exercise

- Now assume that *D* is subjected to surface traction. If

$u_i^0,\ \sigma_{ij}^0$: elastic fields if traction act alone in the absence of eigenstrain

$u_i,\ \sigma_{ij}$: elastic fields due to the eigenstrain prescribed in Ω, then prove that:

$$E_{el} = \frac{1}{2}\int_D \sigma_{ij}^0 u_{i,j}^0\, dV - \frac{1}{2}\int_\Omega \sigma_{ij}\varepsilon_{ij}^*\, dV$$

Hint: Note that

$$E_{el} = \frac{1}{2}\int_D (\sigma_{ij}^0 + \sigma_{ij})(u_{i,j}^0 + u_{i,j} - \varepsilon_{ij}^*)dV$$

Example: Calculation of Elastic Strain Energy of an Edge Dislocation

$$E_{el} = \frac{1}{2}\int_V \sigma_{ij}\varepsilon_{ij}^{(e)}\, dV = -\frac{1}{2}\int_V \sigma_{ij}\varepsilon_{ij}^{(p)}\, dV$$

Elastic strain energy per unit length

$$E_{el} = -\frac{1}{2}\iint_{sphere} 2\sigma_{xy}\varepsilon_{xy}^{(p)}\, dx\, dy = -\iint_{sphere} \frac{\mu b}{2\pi\left(1-\nu\right)} x \frac{x^2-y^2}{r^4}\left(\frac{b}{2}\delta(y)H(-x)\right) dx\, dy$$

$$= -\int_{-R}^{-r_0} \frac{\mu b^2}{4\pi\left(1-\nu\right)}\frac{1}{x}dx = -\frac{\mu b^2}{4\pi\left(1-\nu\right)}\ln x\Big|_{-R}^{-r_0} = \frac{\mu b^2}{4\pi\left(1-\nu\right)}\ln\left(\frac{R}{r_0}\right)$$

Variational Approach

- Remember that

$$\beta^*_{ij}(\vec{r}) = -b_j n_i \delta(\vec{S} - \vec{r})$$

- It can also be written as

$$\beta^{(p)}_{ji} = -b_i n_j \delta(\zeta) H(\eta_0 - \eta)$$

- The ζ axis is along the normal vector ***n***
- the η-axis is along $\boldsymbol{\xi}\times\boldsymbol{n}$.
- η is taken from the dislocation line, where the position is $\eta_0 = \eta_0(l)$.

Variational Approach

- Now consider:

Δx: displacement of the dislocation.

$$\mathrm{d}\beta_{ij}^{(p)} = -b_j n_i \delta(\zeta)\mathrm{d}H(\eta_0 - \eta)$$

- Because $\mathrm{d}H = (\mathrm{d}H / \mathrm{d}\eta_0)\mathrm{d}\eta_0 = \delta(\eta_0 - \eta)\mathrm{d}\eta_0$

$$\hat{n} = \frac{\Delta\vec{x} \times \vec{\xi}}{|\Delta\vec{x}|\sin\phi} \qquad \Delta\eta_0 = \left|\Delta\vec{x}\right|\sin\phi$$

then

$$\Delta\beta_{ij}^{(p)} = -b_j \epsilon_{ilm} \Delta x_l \xi_m \delta(\zeta)\delta(\eta_0 - \eta)$$

The variation in the elastic energy is:

$$\Delta E_{el} = -\int \sigma_{ij} \Delta\beta_{ij}^{(p)} \mathrm{d}V = \sigma_{ij} b_j \epsilon_{ilm} \xi_m \Delta x_l \Delta l$$

Force per unit length is: $F_l = -\dfrac{\partial(E / \Delta l)}{\partial x_l} = -\sigma_{ij} b_j \epsilon_{ilm} \xi_m = \epsilon_{lim} \sigma_{ij} b_j \xi_m$

Force on Dislocations

- The Peach-Koehler force on a dislocation with line direction ξ that is under the external stress $\boldsymbol{\sigma}$ including the stress due to other dislocations reads as

$$\boldsymbol{F} = (\boldsymbol{\sigma} \cdot \boldsymbol{b}) \times \boldsymbol{\xi}.$$

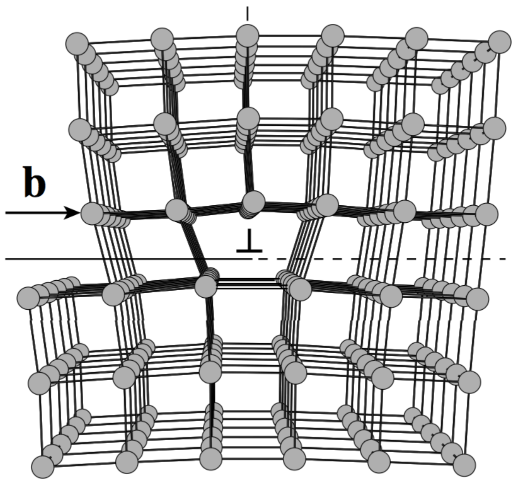
- Note that Peach-Koehler forces are not really Newtonian forces. In fact they are *thermodynamic driving forces*
- It has glide component $\mathrm{F_g}$ and climb component $\mathrm{F_c}$

$$F_g = \boldsymbol{F} \cdot (\boldsymbol{\xi} \times \boldsymbol{m}) \, ,$$

$$F_c = \boldsymbol{F} \cdot \boldsymbol{m}$$

where $\boldsymbol{m} = \boldsymbol{b} \times \boldsymbol{\xi} / |\boldsymbol{b} \times \boldsymbol{\xi}|$ is the unit vector perpendicular to the glide plane of the dislocation

Glide and Climb Components of P-K Force for an Edge Dislocation



[Bulatov & Cai, Computer Simulations of Dislocations]

If $\boldsymbol{b}=[b\ 0\ 0]$ and $\xi=[0\ 0\ 1]$ as shown above. Then and

$$\vec{F} = \begin{bmatrix} b\sigma_{xy} \\ -b\sigma_{xx} \\ 0 \end{bmatrix}.$$

The glide component

$$F_x = F_g = b\sigma_{xy}$$

urges the dislocation to glide in the x-direction and the climb component

$$F_y = -F_c = -b\sigma_{xx}$$

urges the dislocation to climb downward. In this case $\boldsymbol{m} = \boldsymbol{-j}$.

Exercise

- Find the Peach-Koehler force on a screw dislocation