Condensed Matter Physics

Dislocations

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ELTE

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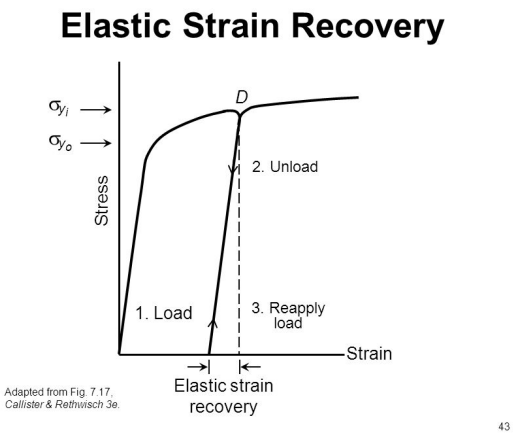
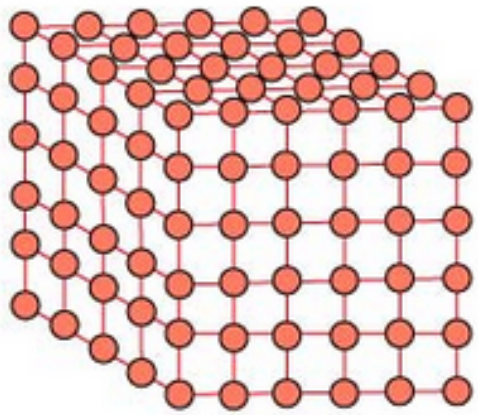
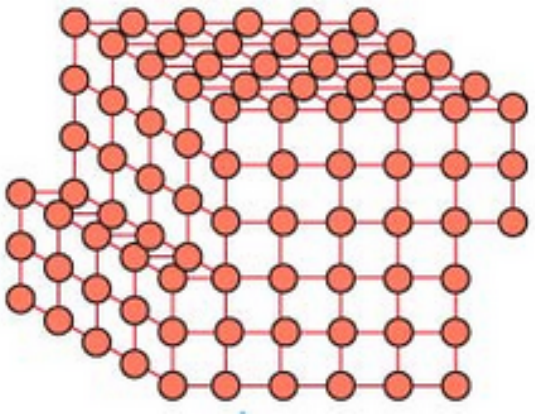
Plastic deformation



Ideal shear





Plastic deformation

Ideal shear

$$F(x) = F_0 \left| \sin\left(\frac{\pi}{a}x\right) \right| = \sigma a^2$$

Small deformation

$$\gamma = \frac{x}{a}, \qquad \sigma = \mu \frac{x}{a}$$

So

$$F_0 = \mu \frac{a^2}{\pi}$$

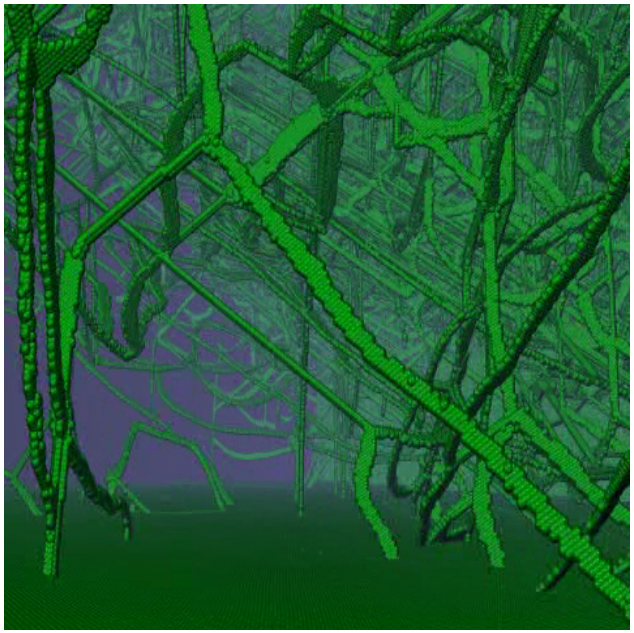
From this

$$\sigma_f \cong \frac{\mu}{\pi} \cong 30 GPa$$

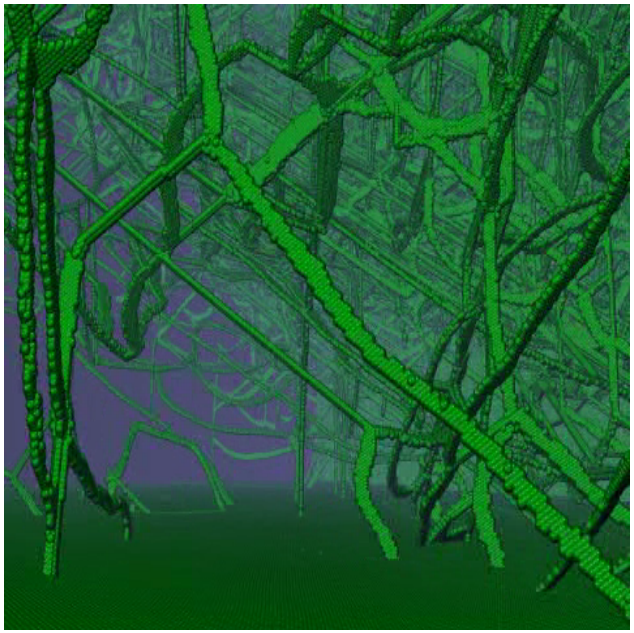
Experiment

$$\sigma_f \cong 100 MPa$$

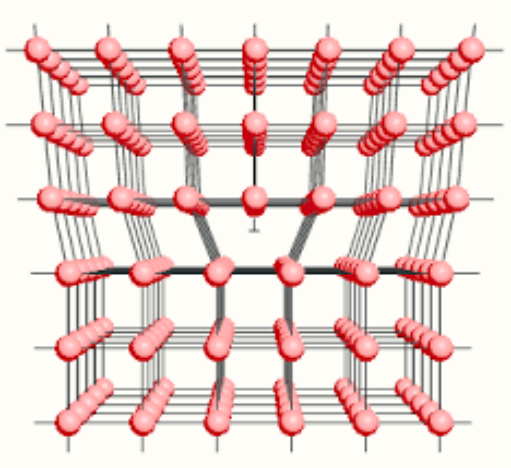
MDD



MDD



Polányi, Orován, Taylor (1934)



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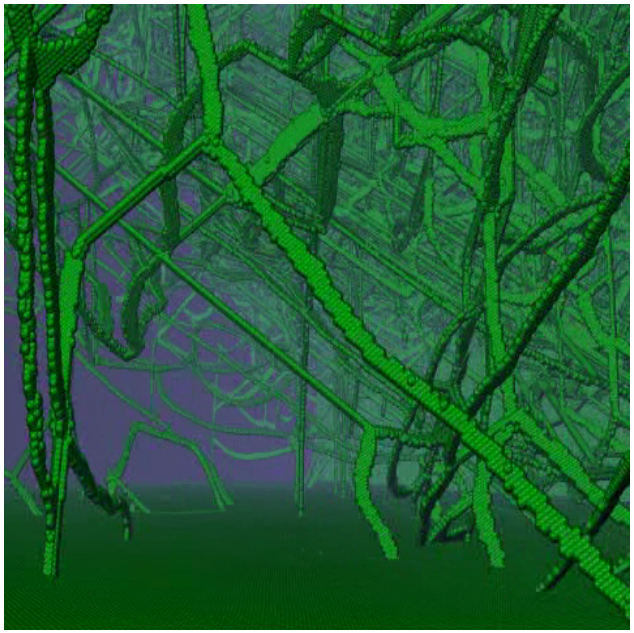

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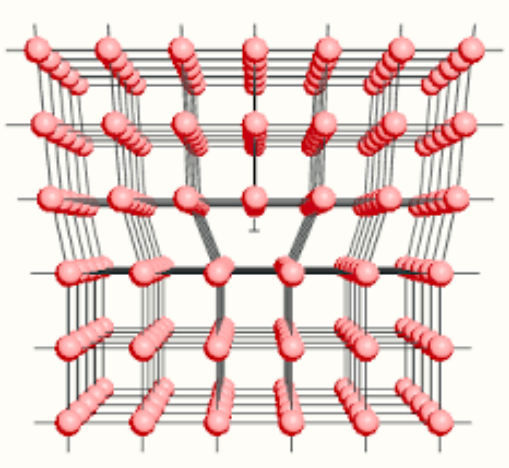
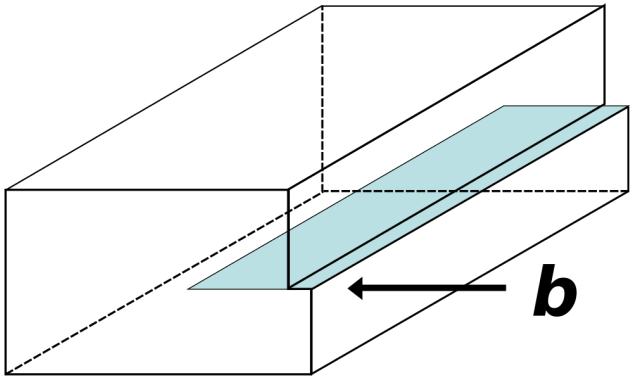


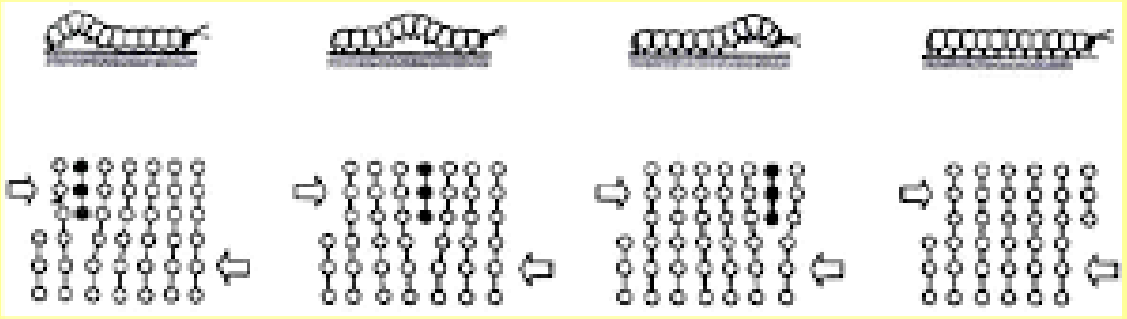
Vito Volterra (1905)



Dislocation

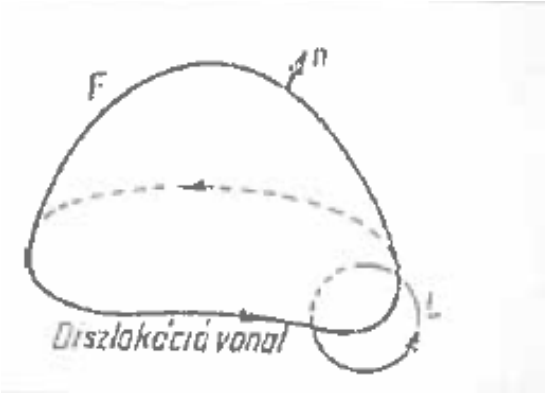
Az elcsúszás nem egyszerre megy végbe

Ez csak akkor lehetséges, ha a kristály tartalmaz egyméretű rácshibákat, diszlokációkat.



Glide: the number of atom is conserved
Climb: the number of atom is not conserved, requires high temperature.

Dislocation



Field theory of dislocations

$$\partial_i u_j := \beta_{ij} = \beta^p_{ij} + \beta^e_{ij} \qquad \frac{d\underline{u}}{d\underline{r}} := \hat{\beta} = \hat{\beta}^e + \hat{\beta}^p$$

Dislocation density tensor

$$\alpha_{ij} = e_{ikl}\partial_k \beta^p_{lj} = -e_{ikl}\partial_k \beta^e_{lj} \qquad \hat{\alpha} = \nabla \times \hat{\beta}^p = -\nabla \times \hat{\beta}^e$$

$$b_j = \int_A \alpha_{ij} dA_i$$

$$b_j = -\int_A e_{ikl} \frac{\partial}{\partial r_k} \beta^e_{lj} dA_i = -\oint \beta^e_{ij} ds_i = -\oint du_j.$$

Dislocation

Individual dislocation

$$\alpha_{ij} = l_i b_j \delta(\xi) \qquad (\hat{\alpha} = \underline{l} \circ \underline{b}\delta(\xi))$$

Plastic distortion

$$\beta^p_{ij}(\vec{r}) = n_i b_k \delta(\zeta)$$

Multiple with the elastic constants and take its div:

$$\frac{\partial}{\partial r_i} C_{ijkl} \frac{\partial u_k}{\partial r_l} = \frac{\partial}{\partial r_i} C_{ijkl} \beta^p_{kl} = f_j \left(div\ \hat{C} \frac{d\underline{u}}{d\underline{r}} = div\ \hat{C}\hat{\beta}^p = \underline{f} \right)$$

Displacement field of a screw dislocation

$$u_3 = \frac{b}{2\pi}\varphi$$

Stress field of a straight dislocation $\sigma \propto b/r$

$$\begin{aligned}
\sigma_{11} &= \frac{\mu b}{2\pi(1-\nu)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2} \\
\sigma_{22} &= \frac{\mu b}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2} \\
\sigma_{12} &= \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}
\end{aligned}$$

Energy of a dislocation

$\sigma \propto b/r$ így $E \propto b^2$

$$2\left(\frac{b}{2}\right)^2 < b^2$$

$$\underline{b} = \underline{a}_i$$

Fcc $\underline{b} = \frac{1}{2}(1,1,0)$
Bcc $\underline{b} = \frac{1}{2}(1,1,1)$

Dislocation-dislocation interaction

Elastic energy

$$E = \frac{1}{2} \int \sigma_{ij} \partial_i u_j dV$$

Let us

$$\sigma_{ij} = \sigma_{ij}^{ext} + \sigma_{ij}^{disl}$$
$$u_i = u_i^{ext} + u_i^{disl}$$

leads to

$$E = \frac{1}{2} \int \left[\sigma_{ij}^{ext} \partial_i u_j^{ext} + \sigma_{ij}^{ext} \partial_i u_j^{disl} + \sigma_{ij}^{disl} \partial_i u_j^{ext} + \sigma_{ij}^{disl} \partial_i u_j^{disl} \right] dV$$

Since

$$\sigma_{ij} = C_{ijkl} \partial_i u_j$$

$$E = E_{ext} + E_{disl} + \int \sigma_{ij}^{ext} \partial_i u_j^{disl} dV$$

Dislocation dislocation interaction

$$E_{int} = \int \sigma_{ij}^{ext} \partial_i u_j^{disl} dV$$

Partial integration

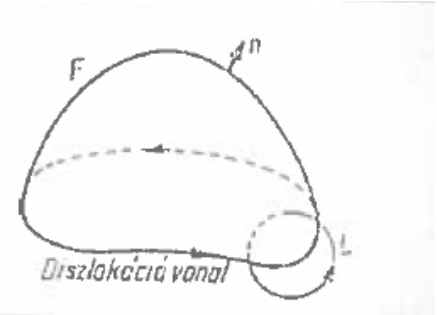
$$E_{int} = \int \partial_i (\sigma_{ij}^{ext} u_j^{disl}) dV - \int (\partial_i \sigma_{ij}^{ext}) u_j^{disl} dV$$

Since

$$\partial_i \sigma_{ij}^{ext} = 0$$

$$E_{int} = \int \partial_i (\sigma_{ij}^{ext} u_j^{disl}) dV = \int (\sigma_{ij}^{ext} u_j^{disl}) dn_i$$

Dislocation-dislocation interaction



$\underline{u}$-nak $\underline{b}$ has a jump on the cut surface!

$$E_{int} = b_j \int_f \sigma_{ij}^{ext} dn_i$$

For the moving line

$$\triangle E_{int} = b_j \oint_v \sigma_{ij}^{ext} (\triangle \underline{r} \times \underline{dl})_i$$

$$\triangle E_{int} = \oint_v (\underline{dl} \times (\hat{\sigma}^{ext} \underline{b}))_i \triangle r_i$$

Peack Koehler force

$$\underline{f} = (\hat{\sigma}^{ext} \underline{b}) \times \underline{l}$$

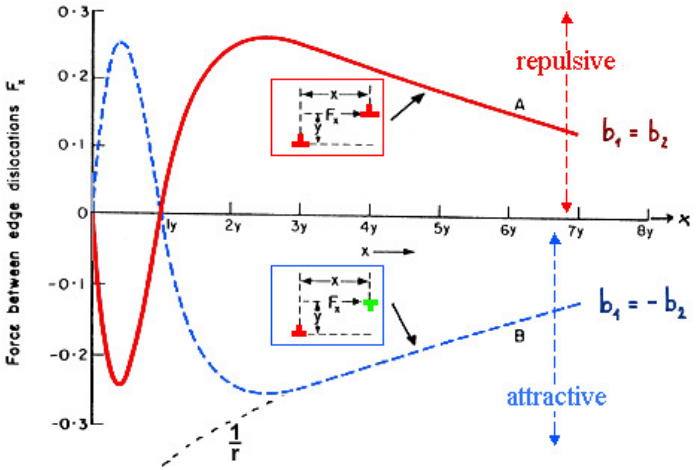
Dislocation-dislocation interaction

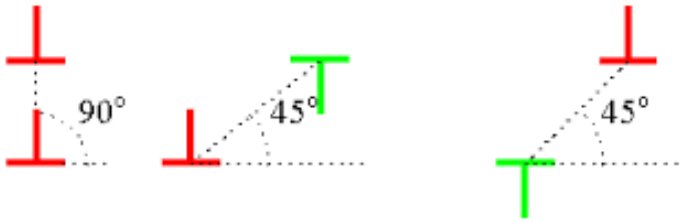
For glide only, we need

$$f_{glide} = [(\hat{\sigma}^{ext}\underline{b}) \times \underline{l}]\frac{b}{\overline{b}} = \underline{n}\hat{\sigma}^{ext}\underline{b} = \tau b \text{ ahol } \underline{n} = \frac{b}{\overline{b}} \times \underline{l}$$

Edge dislocation

$$f = b_1 b_2 \frac{\mu}{2\pi(1-\nu)} \frac{x(x^2-d^2)}{(x^2+d^2)^2}$$

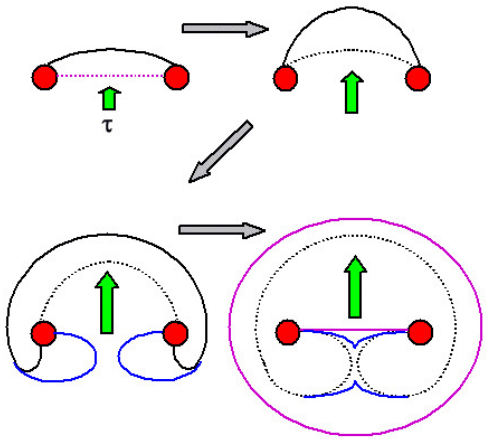




Possible equilibrium configurations

Dislocation multiplication

Frank-Read source

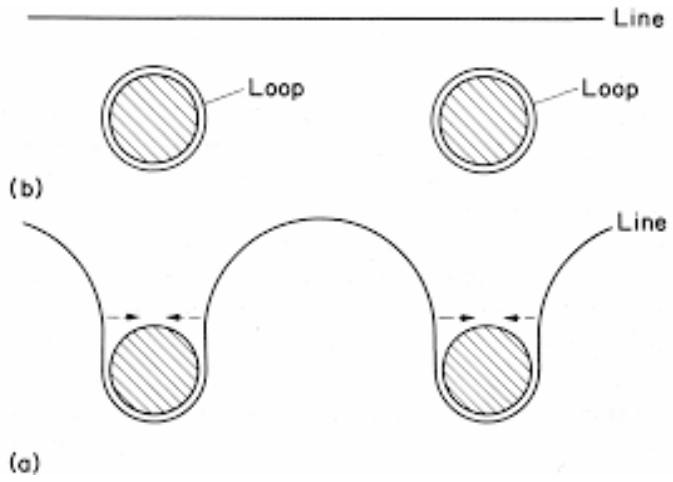


Flow stress (Taylor relation)

$$\tau_f = \alpha \mu b \sqrt{\rho}$$

Work hardening by precipitate

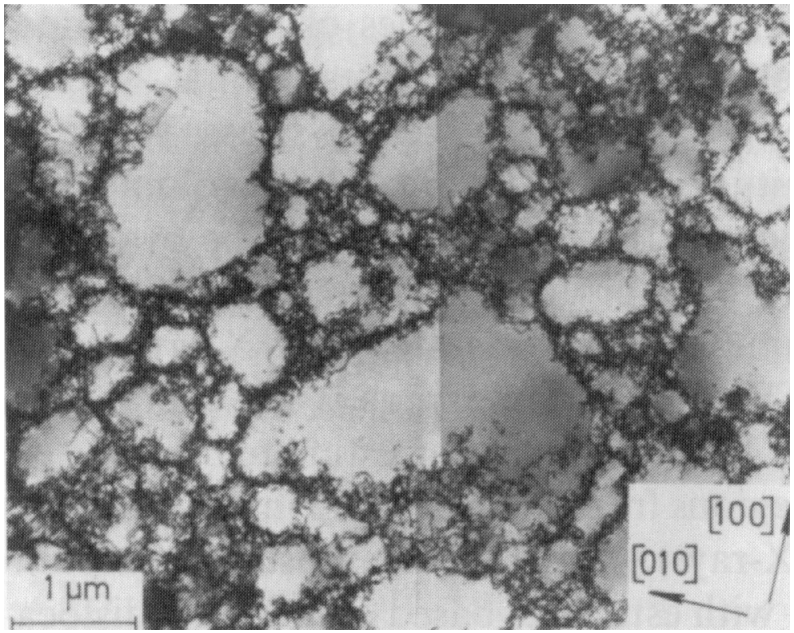
Line tension $\tau_l = E_l/R$



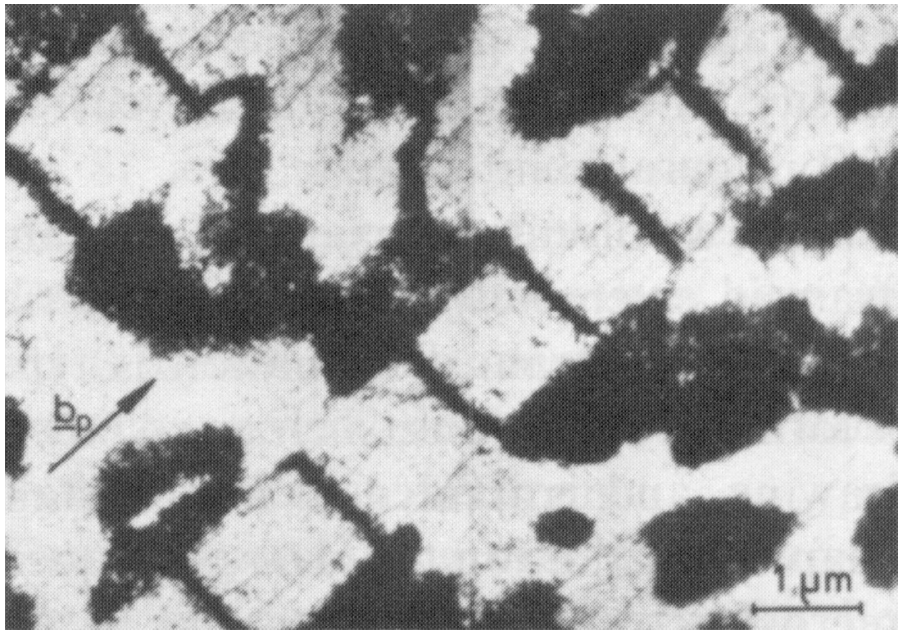
Critical stress

$$\tau_c = \propto \frac{1}{l}$$

Dislocation patterning

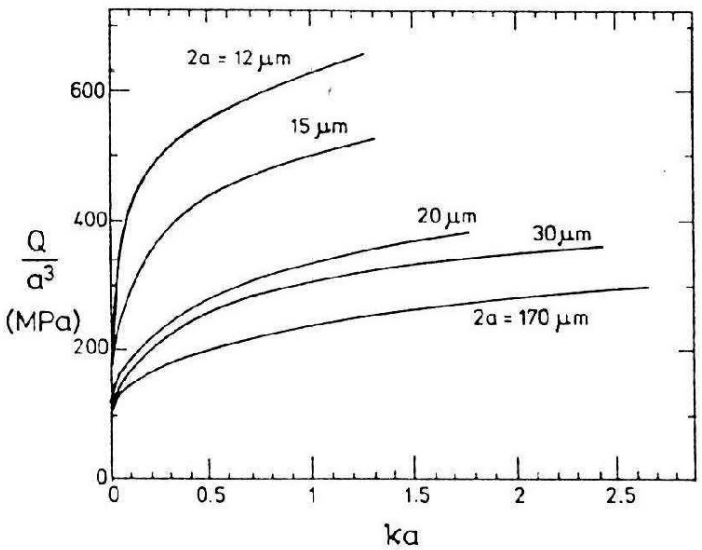


Cell structure

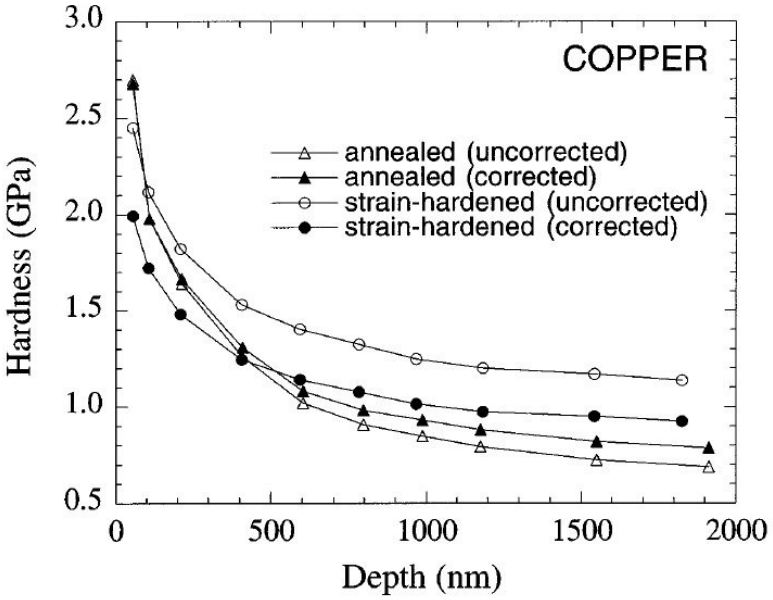


PSB structure

Size effect

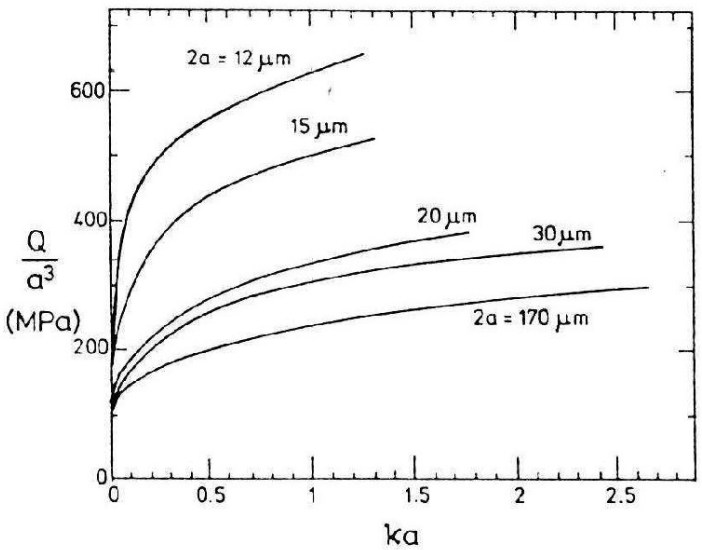


Torsion test

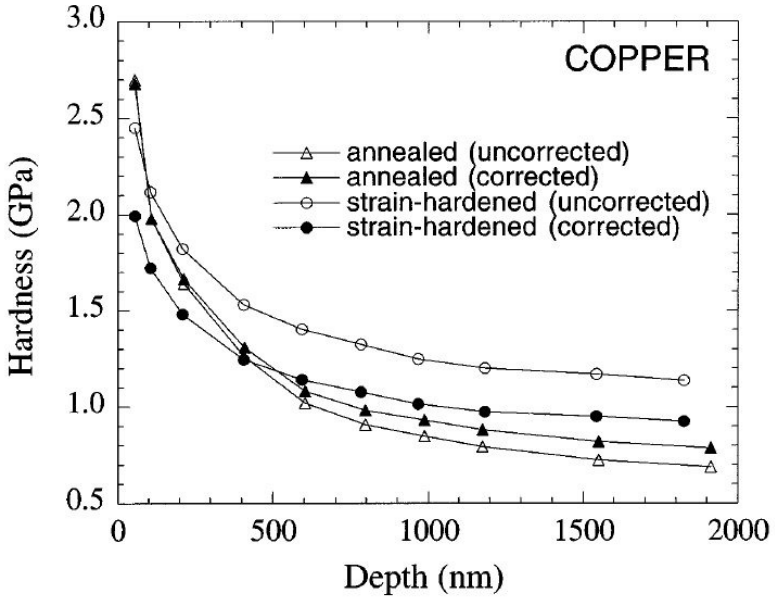


Microhardness

Size effect



Torsion test

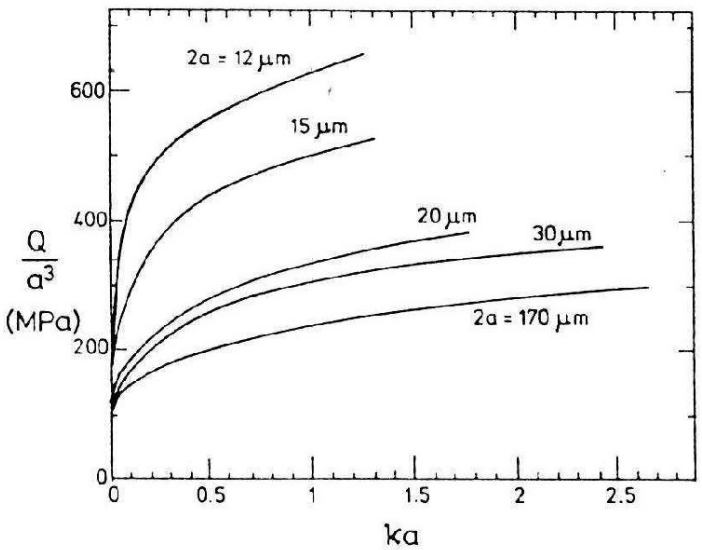


Microhardness

Local plasticity

$$\tau_{class}(\gamma, \dot{\gamma}, \ldots)$$

Size effect



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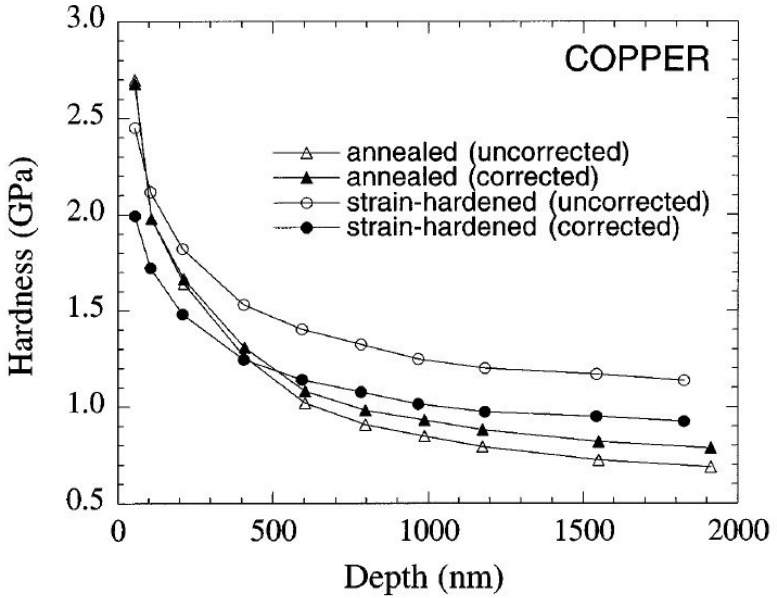
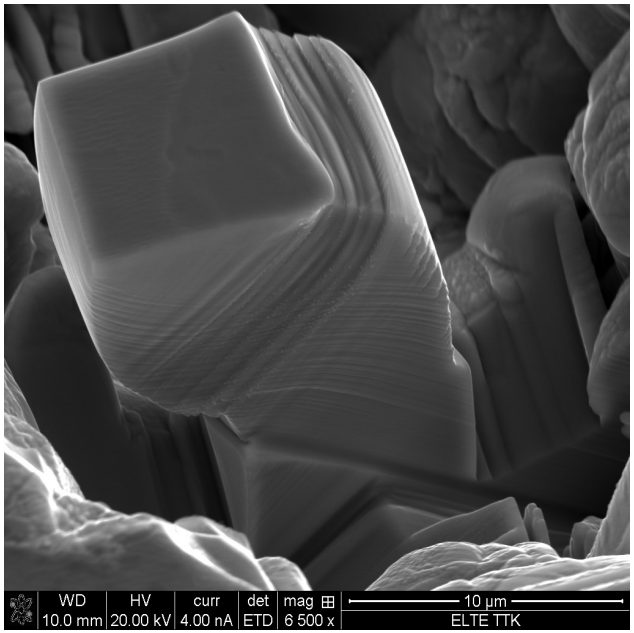


Microhardness

Nonlocal plasticity

$$\tau(\gamma, \dot{\gamma}, ...) = \tau_{class}(\gamma, \dot{\gamma}, ...) + l^2 \mu \frac{d^2}{d\vec{r}^2} \gamma$$

Pillar compression



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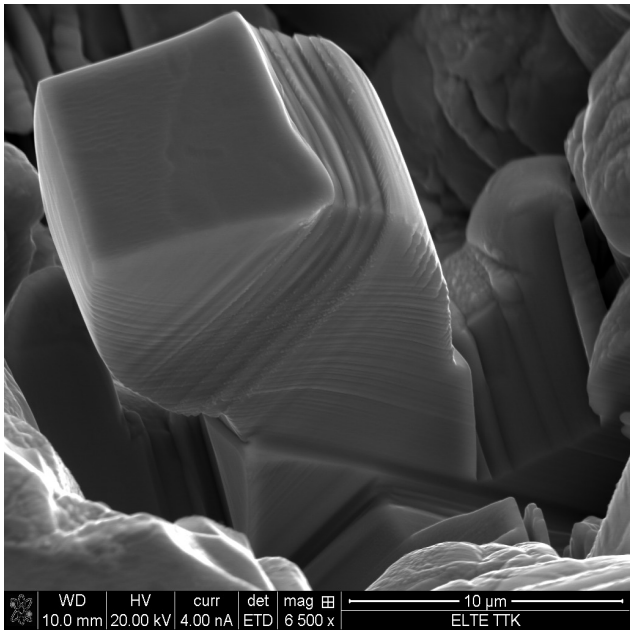

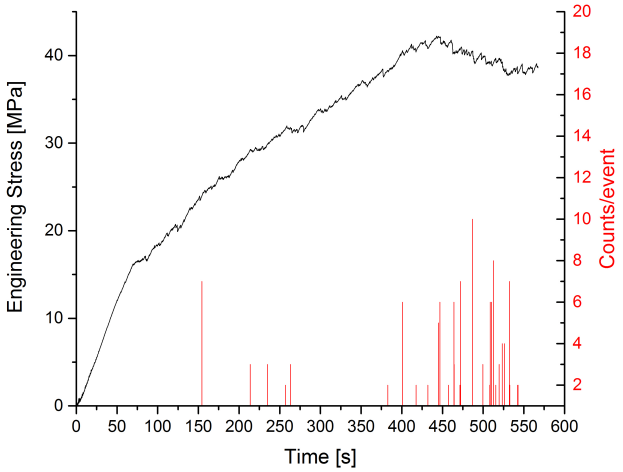

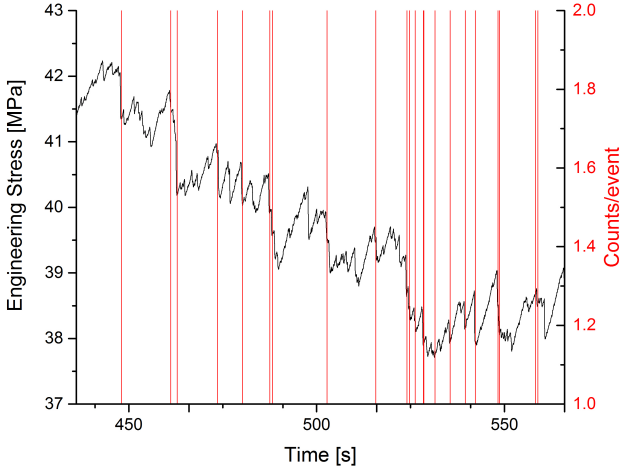

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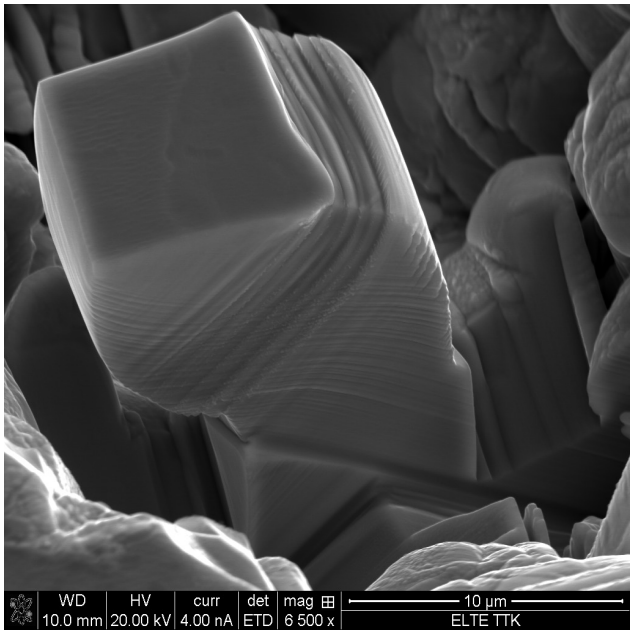

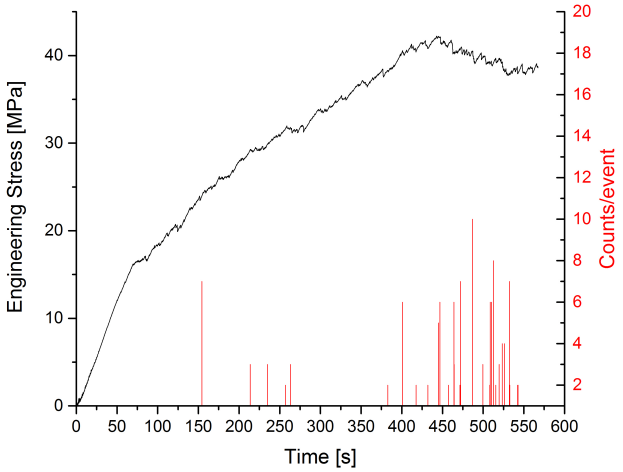

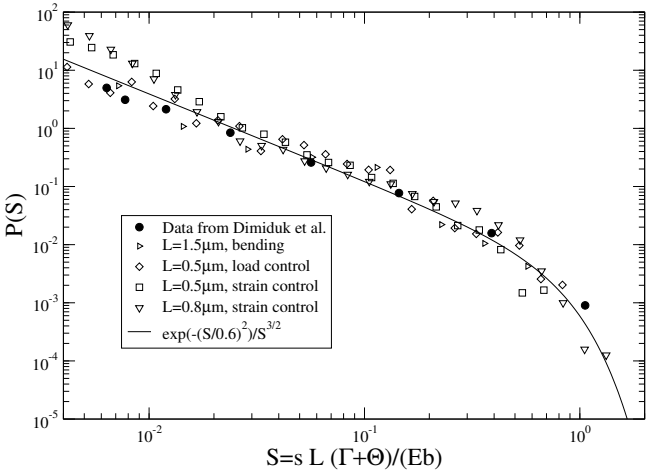

Relevant quantities

Plastic deformation

$$\frac{d\vec{R}}{d\vec{r}} = \hat{1} + \frac{d\vec{u}}{d\vec{r}} = \hat{F}^e \cdot \hat{F}^p$$

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Plastic deformation

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Definitions

$$\hat{F}^{e,p} = \hat{1} + \hat{\beta}^{e,p}$$

$$\hat{F}^e \cdot \hat{F}^{e*} = \hat{1} + 2\hat{\epsilon}^e$$

$$Curl\hat{F}^p = \hat{\alpha}$$

Small deformations

Deformations

$$\partial_i u_j := \beta_{ij} = \beta^p_{ij} + \beta^e_{ij} \qquad \frac{d\vec{u}}{d\vec{r}} := \hat{\beta} = \hat{\beta}^e + \hat{\beta}^p$$

Nye's dislocation density tensor

Small deformations

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Is it that we learned in school?

$$b_j = \int_A \alpha_{ij} dA_i$$

$$b_j = -\int_A e_{ikl} \frac{\partial}{\partial r_k} \beta_{lj} dA_i = -\oint \beta_{ij} ds_i = -\oint du_i.$$

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Deformations

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$$b_j = -\int_A e_{ikl} \frac{\partial}{\partial r_k} \beta_{lj} dA_i = -\oint \beta_{ij} ds_i = -\oint du_i.$$

For a single dislocation

$$\alpha_{ij} = l_i b_j \delta(\xi) \qquad \left(\hat{\alpha} = \vec{l} \circ \vec{b}\delta(\xi)\right)$$

Incompatibility

Incompatibility operator

$$(Inc\hat{A})_{ij} = -e_{ikm}e_{jln}\partial_k\partial_l A_{mn} \qquad Inc\hat{A} = -\nabla \times \hat{A} \times \nabla$$

$$Inc(\partial_i f_j + \partial_j f_i) \equiv 0 \qquad Inc\left[\frac{d\vec{f}}{d\vec{r}}\right]_{sim} \equiv 0$$

Incompatibility

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Incompatibility field

$$\eta_{ij} = -e_{ikm}e_{jln}\frac{\partial}{\partial r_k}\frac{\partial}{\partial r_l}\epsilon^e_{mn} \qquad \left(inc\,\hat{\epsilon}^e = \hat{\eta}\right)$$

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Incompatibility field

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$$\eta_{ij} = \frac{1}{2}\left(e_{jln}\frac{\partial}{\partial r_l}\alpha_{im} + e_{iln}\frac{\partial}{\partial r_l}\alpha_{jm}\right) \qquad \left(\hat{\eta} = [\hat{\alpha} \times \nabla]_{sym}\right)$$

Stress

Linear elasticity

$$\sigma_{ij} = L_{ijkl}\epsilon^e_{kl} \qquad \left(\hat{\sigma} = \hat{L} : \hat{\epsilon}^e\right)$$

Stress

Linear elasticity

$$\sigma_{ij} = L_{ijkl}\epsilon^e_{kl} \qquad \left(\hat{\sigma} = \hat{L} : \hat{\epsilon}^e\right)$$

Elastic deformation $\leftrightarrow$ Stress

$$\eta_{ij} = -e_{ikm}e_{jln}\frac{\partial}{\partial r_k}\frac{\partial}{\partial r_l}L^{-1}_{mnop}\sigma_{op} \qquad \left(inc\left(\hat{L}^{-1}\hat{\sigma}\right) = \hat{\eta}\right)$$

Stress

Linear elasticity

$$\sigma_{ij} = L_{ijkl}\epsilon^e_{kl} \qquad \left(\hat{\sigma} = \hat{L} : \hat{\epsilon}^e\right)$$

Elastic deformation $\leftrightarrow$ Stress

$$\eta_{ij} = -e_{ikm}e_{jln}\frac{\partial}{\partial r_k}\frac{\partial}{\partial r_l}L^{-1}_{mnop}\sigma_{op} \qquad \left(inc\left(\hat{L}^{-1}\hat{\sigma}\right) = \hat{\eta}\right)$$

Is it enough?

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Equilibrium condition

$$\frac{\partial}{\partial r_i}\sigma_{ij} = 0 \qquad (div\ \hat{\sigma} = 0)$$

Second order stress function

$$\sigma_{ij} = -e_{ikm} e_{jln} \frac{\partial}{\partial r_k} \frac{\partial}{\partial r_l} \chi_{mn} \qquad (\hat{\sigma} = inc\ \hat{\chi})$$

Second order stress function

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Due to the identity

$$div\ inc \equiv 0 \qquad div\ \hat{\sigma} = 0$$

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$$\eta_{ij} = e_{ikm} e_{jln} e_{oqv} e_{puw} L^{-1}_{mnop} \frac{\partial}{\partial r_k} \frac{\partial}{\partial r_l} \frac{\partial}{\partial r_q} \frac{\partial}{\partial r_u} \chi_{vw} \qquad \left(\hat{\eta} = inc \left(\hat{L}^{-1} inc\, \hat{\chi}\right)\right)$$

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for isotropic materials

$$\begin{aligned} \chi'_{ij} &= \frac{1}{2\mu}\left(\chi_{ij} - \frac{\nu}{1+2\nu}\chi_{kk}\delta_{ij}\right) \\ \chi_{ij} &= 2\mu\left(\chi'_{ij} + \frac{\nu}{1-\nu}\chi'_{kk}\delta_{ij}\right) \end{aligned}$$

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$$\nabla^4 \chi'_{ij} = \eta_{ij} \qquad \left(\nabla^4 \hat{\chi}' = \hat{\eta}\right).$$

gauge condition

$$\frac{\partial}{\partial r_i} \chi'_{ij} = 0 \qquad (div\ \hat{\chi}' = 0)$$

2D case

Stress function $\rightarrow$ stress ($\partial/\partial z = 0$)

$$\sigma_{11} = -\frac{\partial^2 \chi}{\partial y^2}, \qquad \sigma_{22} = -\frac{\partial^2 \chi}{\partial x^2}, \qquad \sigma_{12} = \frac{\partial^2 \chi}{\partial x \partial y}, \qquad \chi \equiv \chi_{33}$$

$$\sigma_{23} = -\frac{\partial \phi}{\partial x}, \qquad \sigma_{13} = \frac{\partial \phi}{\partial y}, \qquad \phi = -\frac{\partial \chi_{23}}{\partial x} + \frac{\partial \chi_{31}}{\partial y}$$

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Field equations

Edge dislocation

$$\nabla^4 \chi = \frac{2\mu}{1-\nu}\left(b_1 \frac{\partial}{\partial y} - b_2 \frac{\partial}{\partial x}\right)(\rho_{d+} - \rho_{d-})$$

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Shrew dislocation

$$\nabla^2 \phi = \mu b_3 (\rho_{d+} - \rho_{d-})$$

2D stress

$$\nabla^4 G = \delta(r) \quad G(\vec{r}) = \frac{1}{8\pi} r^2 \ln(r)$$

$$\begin{aligned}
\sigma_{11} &= \frac{\mu b}{2\pi(1-\nu)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2} \\
\sigma_{22} &= \frac{\mu b}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2} \\
\sigma_{12} &= \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}
\end{aligned}$$

Variational approaches I.

Classical elasticity $F(\hat{\epsilon}) = F(\left[d\vec{u}/d\vec{r}\right]_{sim}$

$$\hat{\sigma} = \frac{\delta F}{\delta \epsilon}$$

$$\frac{\delta F}{\delta u_i} = \partial_j \frac{\delta F}{\delta \epsilon_{ij}} = \partial_j \sigma_{ij} = 0$$

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Plasticity

$$Q[\hat{\epsilon}_e, \hat{\chi}] = F(\hat{\epsilon}) - \int [\hat{\chi} : (Inc\hat{\epsilon}^e - \hat{\eta})] dV$$

$$\frac{\delta Q}{\delta \hat{\epsilon}^e} = \hat{\sigma} - Inc\hat{\chi} = 0, \qquad \frac{\delta Q}{\delta \hat{\chi}} = Inc\hat{\epsilon}^e - \hat{\eta} = 0$$

Variational approaches II.

Gibbs free energy $G(\hat{\sigma})$

$$-\frac{\delta G}{\delta \hat{\sigma}} = \hat{\epsilon}^{e}$$

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Consider

$$P[\hat{\chi}] = G(Inc\hat{\chi} = \hat{\sigma}) + \int [\hat{\chi} : \hat{\eta})] dV$$

One obtains

$$\frac{\delta P}{\delta \hat{\chi}} = Inc\frac{\delta G}{\delta \hat{\sigma}} + \hat{\eta} = -Inc\hat{\epsilon}^e + \hat{\eta} = 0,$$

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Dislocation dislocation interaction (Peach-Koehler force)

$$F_i = e_{ikl} t_k \sigma_{lm} b_m = -\frac{dP}{dr_i^j}$$

Plain strain (2D) case

$$P[\chi] = \int \left[-\frac{D}{2}(\triangle\chi)^2 + b\chi\partial_y\kappa) \right] dV$$

with $D = (1-\nu)/2\mu$, and

$$\kappa = \sum_j \pm\delta(\vec{r} - \vec{r}_j)$$

Leading to

$$D \triangle^2 \chi = b\partial_y \left[\sum_j \pm\delta(\vec{r} - \vec{r}_j) \right]$$

Core regularization

Nonlocal term

$$G_{\text{nonlocal}}[\sigma] = G_0 - b^2 \int N_{ijklmn}(\partial_i \sigma_{jk})\partial_l \sigma_{mn} \mathrm{d}V,$$

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2D isotopic material

$$P[\chi] = \int \left\{ -\frac{1-\nu}{4\mu} \left[|\triangle\chi|^2 + a^2 |\nabla\triangle\chi|^2 \right] + bchi\partial_2 \delta(\boldsymbol{r}) \right\} \mathrm{d}^2 r$$

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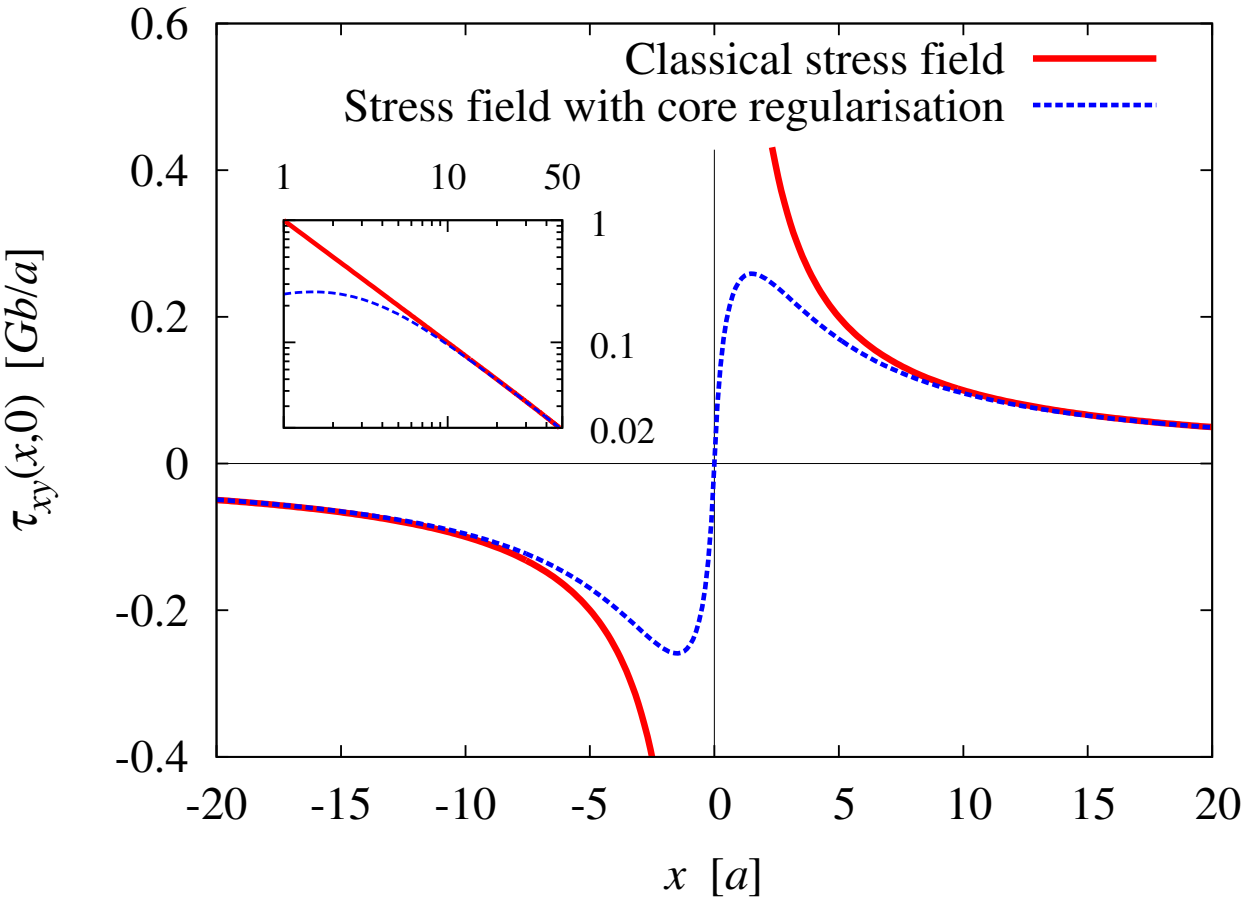
Leading To

$$\triangle^2\chi - a^2\triangle^3\chi = \frac{2b\mu}{1-\nu}\partial_2\delta(\boldsymbol{r})$$

$$\chi = \frac{ba}{4\pi D}\frac{y}{r}\left[-2K_1\left(\frac{r}{a}\right) + 2\frac{a}{r} + \frac{r}{a}\ln\left(\frac{r}{a}\right)\right]$$

Core regularization



Role of elastic anharmonicity

$$\sigma_{ij} = L_{ijkl}\epsilon_{kl} + K_{ijklmn}\epsilon_{kl}\epsilon_{mn}$$

Role of elastic anharmonicity

$$G_{\mathrm{anharm}}[\sigma] := G_0 + \int \left[C_{ijklmn}\sigma_{ij}\sigma_{kl}\sigma_{mn} + \mathcal{O}(\sigma_{ij}^4) \right] \mathrm{d}V$$

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2D edge dislocation

$$G[\chi] := \int \left[-\frac{D}{2}(\triangle\chi)^2 + \epsilon_{\mathrm{a}}\frac{D^2}{3}(\triangle\chi)^3 \right] \mathrm{d}^2$$

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Extra energy

$$V_1(\boldsymbol{r}) = \frac{(b_1 - b_2)b^2}{16\pi^2 D} \left[\frac{y(3x^2 + y^2)}{r^4} + 4\frac{y}{r^2} \ln\left(\frac{r}{r_0}\right) \right].$$

Time evolution

Dislocation density tensor

$$\alpha_{ij} = e_{ikl} \frac{\partial}{\partial r_k} \beta^p_{lj} \qquad \left(\hat{\alpha} = \nabla \times \hat{\beta}^p\right)$$

Time evolution

Evolution equation

$$\dot{\alpha}_{ij} + e_{ikl}\frac{\partial}{\partial r_k} j_{lj} = 0 \qquad \left(\dot{\hat{\alpha}} + \nabla \times \hat{j} = 0\right)$$

where

$$\hat{j} = -\dot{\hat{\beta}}^p$$

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Physical meaning

$$\frac{db_j}{dt} = -\oint_L j_{ij} ds_i$$

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Physical meaning

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For individual dislocation (Orowan's equation)

$$j_{ik} = e_{ilm} l_l v_m b_k \delta(\xi) \qquad \left(\hat{j} = (\vec{l} \circ \vec{b}\delta(\xi)) \times \vec{v}\right)$$

Displacement field

Plastic deformation

$$\frac{\partial u_j}{\partial r_i} = \beta^e_{ij} + \beta^p_{ij} \qquad \left(\frac{d\vec{u}}{d\vec{r}} = \hat{\beta}^e + \hat{\beta}^p\right)$$

Displacement field

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$$\frac{\partial u_j}{\partial r_i} = \beta^e_{ij} + \beta^p_{ij} \qquad \left(\frac{d\vec{u}}{d\vec{r}} = \hat{\beta}^e + \hat{\beta}^p\right)$$

Multiply with $\hat{L}$ and take its *div*

$$\frac{\partial}{\partial r_i} L_{ijkl} \frac{\partial u_k}{\partial r_l} = \frac{\partial}{\partial r_i} L_{ijkl} \beta^p_{kl} \qquad \left(div\ \hat{L} \frac{d\vec{u}}{d\vec{r}} = div\ \hat{L}\hat{\beta}^p\right)$$

Displacement field

Plastic deformation

$$\frac{\partial u_j}{\partial r_i} = \beta^e_{ij} + \beta^p_{ij} \qquad \left(\frac{d\vec{u}}{d\vec{r}} = \hat{\beta}^e + \hat{\beta}^p\right)$$

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Taking the time derivative

$$\frac{\partial}{\partial r_i} L_{ijkl} \frac{\partial \dot{u}_k}{\partial r_l} = \frac{\partial}{\partial r_i} L_{ijkl} j_{kl} \qquad \left(div\ \hat{L} \frac{d\dot{\vec{u}}}{d\vec{r}} = div\ \hat{L}\hat{j}\right)$$