Continuum dislocation theory: size effects and formation of microstructure

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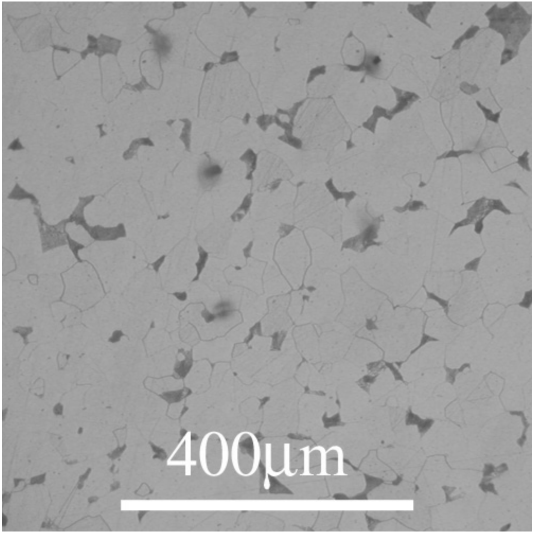
Outline of my lecture

- Size effects in crystal plasticity and formation of microstructure
- Why continuum dislocation theory?
- Thermodynamic framework of CDT
- Antiplane constrained shear
- Plane constrained shear
- Double slip systems
- Mechanism of twin formation
- Continuum model of deformation twinning
- Bending
- Polygonization
- Conclusion
- Further works

Size effects in crystal plasticity and formation of microstructures

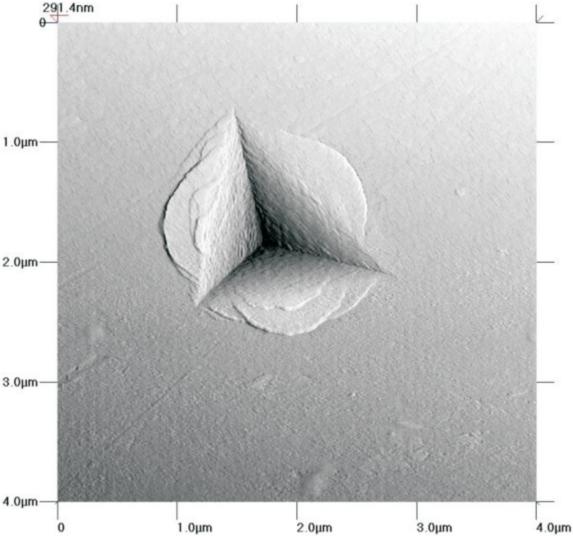
- Hall-Petch relation
- Indentation
- Shear, torsion, bending
- Deformation twinning
- Polygonization
- Recrystallization
- Grain growth
- Texturing
- ect.

Hall-Petch relation



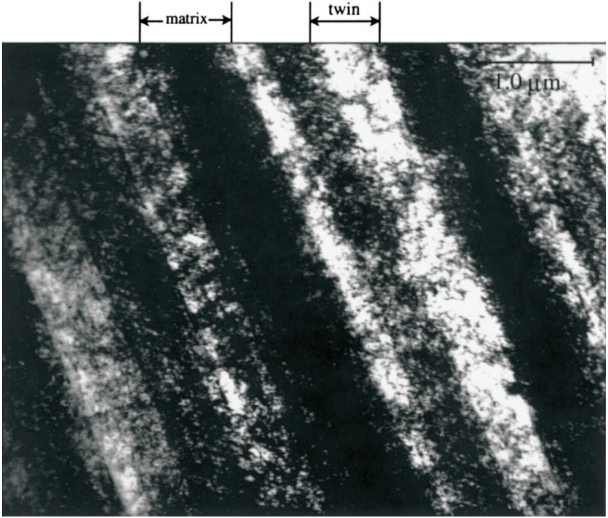
$$\sigma_Y \propto \sigma_{Y0} + \frac{\lambda}{\sqrt{d}}$$

Indentation test



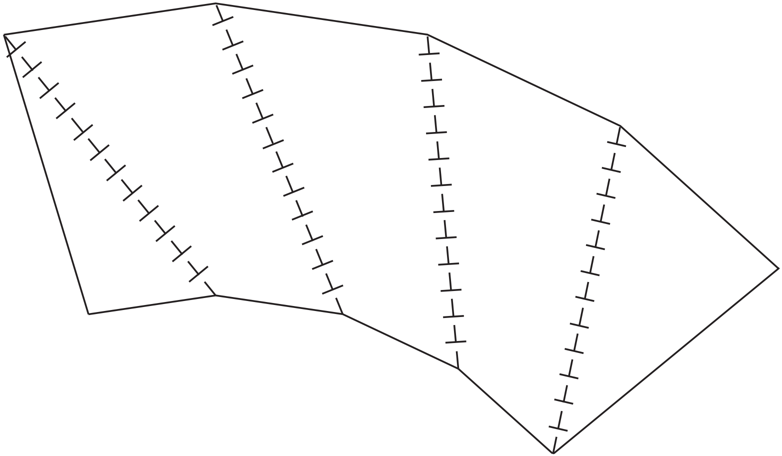
$$H = \frac{F}{A} \quad \text{(Hardness)}$$

Twin formation

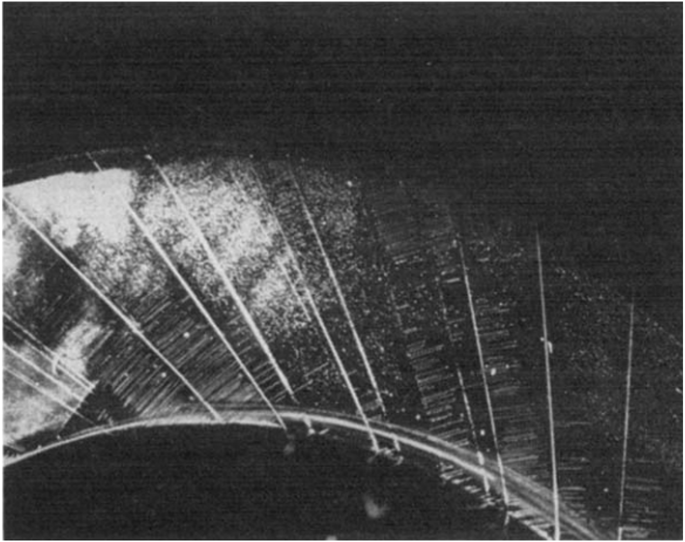


TEM micrograph of the $[\bar{1}11]$ oriented single crystal under tension. Strain 30%, Karaman et al., 2000

Polygonization



Polygonized state of a bent single crystal beam



View along intersections of slip planes with polygon boundaries in a polygonized zinc crystal, Gilman, 1955

Why continuum dislocation theory?

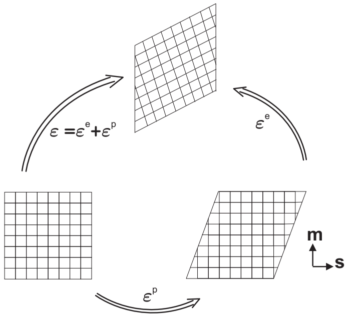
- Plastic deformations are due to nucleation, multiplication and motion of dislocations
- Dislocations appear to reduce energy of crystals
- Motion of dislocations produces energy dissipation which causes the resistance to their motion
- Under favorable condition the rearrangement of dislocations by dislocation climbing and gliding may reduce further energy of crystals
- Deformation twinning and polygonization are low energy dislocation structures
- Continuum description is dictated by high dislocation densities (10^8-$10^{14}\mathrm{m}^{-2}$). To compare: dislocation density $4\times 10^{11}\mathrm{m}^{-2}$ means that the total length of dislocation loops in one cubic meter of crystal equals the distance from the earth to the moon

Related literature

- Continuum dislocation theory: Kondo,1952; Nye,1953; Bilby *et al.*,1955; Kröner,1955,1958; Berdichevsky & Sedov,1967; Le & Stumpf,1996a,b,c; Ortiz & Repetto,1999; Ortiz *et al.*,2000; Acharya,2001; Svendsen,2002; Gurtin,2002,2004; Berdichevsky,2006; Berdichevsky & Le,2007; Le & Sembiring,2008a,b,2009; Kochmann & Le,2008,2009a,b; Le &Nguyen,2010,2011; Le & Nguyen,2012.
- Strain gradient plasticity: Fleck *et al.*,1994; Shu & Fleck,1999; Gao *et al.*,1999; Acharya & Bassani,2000; Huang *et al.*,2000,2004; Fleck & Hutchinson,2001; Han *et al.*,2005; Aifantis & Willis,2005.
- Statistical mechanics of dislocations: Le & Berdichevsky,2001,2002; Groma *et al.*,2003,2005; Berdichevsky,2005,2006.
- Discrete dislocation simulations: Needleman & Van der Giessen,2001; Shu *et al.*,2001; Yefimov *et al.*,2004.

Thermodynamic framework of CDT

Kinematics



Small strain theory: unknown functions $u_i(x), \beta_{ij}(x)$

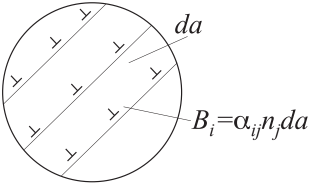
Plastic distortion: $\beta_{ij} = \sum_{\mathfrak{a}=1}^{n} \beta_{\mathfrak{a}}(x) s_i^{\mathfrak{a}} m_j^{\mathfrak{a}}$

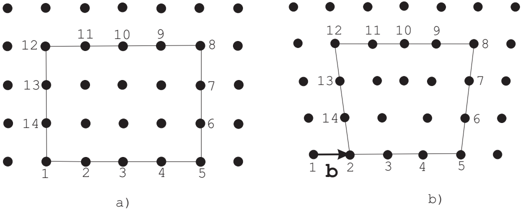
Total (compatible) strain: $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$

Plastic (incompatible) strain: $\varepsilon_{ij}^{p} = \frac{1}{2}(\beta_{ij} + \beta_{ji})$

Elastic (incompatible) strain: $\varepsilon_{ij}^{e} = \varepsilon_{ij} - \varepsilon_{ij}^{p}$

Dislocation density





Dislocation density: $\alpha_{ij} = \epsilon_{jkl}\beta_{il,k}$

Geometrical interpretation: Stokes theorem

$$\int_{\mathcal{S}} \alpha_{ij} n_j \, da = \oint_{\mathcal{L}} \beta_{ij} \tau_j \, ds = B_i$$

B_i is the resultant Burgers vector of all GND (excess dislocations), whose dislocation lines cuts the area $\mathcal{S}$. For single slip the scalar dislocation density is $\rho = \frac{1}{b}|\epsilon_{jkl}\beta_{,k} m_l n_j|$.

Energetics

State variables: elastic strain ε^e_{ij} and dislocation density α_{ij} (plastic strain and its gradient are history dependent and are not the state variables)

Free energy density (Kröner)

$$\psi(\varepsilon_{ij} - \varepsilon^p_{ij}, \alpha_{ij}) = \psi_0(\varepsilon_{ij} - \varepsilon^p_{ij}) + \psi_m(\alpha_{ij})$$

Elastic energy of the crystal lattice

$$\psi_0(\varepsilon^e_{ij}) = \frac{1}{2} C_{ijkl} \varepsilon^e_{ij} \varepsilon^e_{kl}$$

Energy of microstructure (single slip system, Berdichevsky, 2006)

$$\boxed{\psi_m(\alpha_{ij}) = \mu k \ln \frac{1}{1 - \rho/\rho_s}}$$

Small up to moderate dislocation density

$$\psi_m(\alpha_{ij}) \simeq \mu k \left(\frac{\rho}{\rho_s} + \frac{1}{2} \frac{\rho^2}{\rho_s^2} \right)$$

Variational principles of CDT

Negligible resistance to dislocation motion: the energy minimization

$$I(u_i, \beta_{ij}) = \int_\Omega \psi(\varepsilon_{ij} - \varepsilon^p_{ij}, \alpha_{ij}) dx \to \min_{u,\beta}$$

Finite resistance to dislocation motion: Variational equation (Sedov, Berdichesky, 1967)

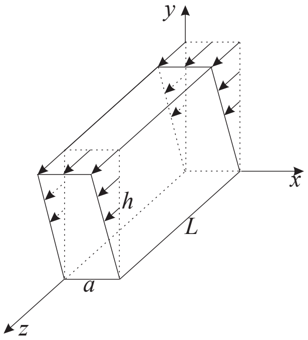
$$\delta I + \int_\Omega \frac{\partial D}{\partial \dot{\beta}_{ij}} \delta\beta_{ij}\, dx = 0$$

implying the evolution equation (of Biot type) for the plastic distortion

$$\frac{\partial D}{\partial \dot{\beta}_{ij}} = -\frac{\delta_\varepsilon \psi}{\delta \beta_{ij}} \equiv -\frac{\partial \psi}{\partial \beta_{ij}} + \frac{\partial}{\partial x_k} \frac{\partial \psi}{\partial \beta_{ij,k}}$$

Note that, if the dissipation potential $D = D(\dot{\beta}_{ij})$ is a homogeneous function of first order (rate-independent theory), the variational equation reduces to the minimization of "relaxed" energy.

Antiplane constrained shear



A single crystal strip is placed in a "hard" device with the prescribed displacements at the boundary

$$u_z = \gamma y$$

γ overall shear strain (control parameter)
Assumption: $a \ll h, a \ll L$

Single slip system

Plastic distortion

$$\beta_{zy} = \beta(x)$$

Since dislocation cannot reach the boundary $x = 0, a$, the plastic distortion $\beta(y)$ satisfies the constraints:

$$\beta(0) = \beta(a) = 0$$

The plastic strains are given by

$$\varepsilon^p_{yz} = \varepsilon^p_{zy} = \frac{1}{2}\beta(x).$$

The only non-zero component of tensor of dislocation density is

$$\alpha_{zz} = \beta_{,x}.$$

The free energy density of the crystal with dislocations takes a simple form

$$\psi = \frac{1}{2}\mu(\gamma - \beta)^2 + \mu k(\frac{|\beta_{,x}|}{\rho_s b} + \frac{\beta^2_{,x}}{\rho^2_s b^2}),$$

Energy minimization

If the resistance to dislocation motion is negligible, the true plastic distortion minimizes the total energy

$$I[\beta(x)] = hL \int_0^a \left[\frac{1}{2}\mu(\gamma - \beta)^2 + \mu k \left(\frac{|\beta_{,x}|}{\rho_s b} + \frac{\beta_{,x}^2}{\rho_s^2 b^2} \right) \right] dx$$

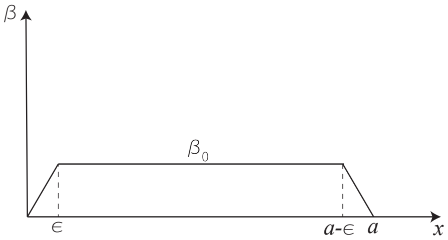
Introducing the dimensionless quantities

$$\bar{x} = x b \rho_s, \quad \bar{a} = a b \rho_s, \quad E = \frac{b\rho_s}{\mu h L} I$$

to rewrite the energy functional in the form

$$E[\beta(x)] = \int_0^a \left[\frac{1}{2}(\gamma - \beta)^2 + k \left(|\beta'| + \frac{1}{2}\beta'^2 \right) \right] dx$$

Energetic threshold



$$E = \frac{1}{2}(\gamma - \beta_0)^2 a + 2k|\beta_0|$$

Minimization of this function shows that there exists the threshold value

$$\boxed{\gamma_{en} = \frac{2k}{ab\rho_s}}$$

Size effect (typical to all gradient theories): the threshold value is inversely proportional to the size a of the specimen.

Minimizer

Ansatz (based on the feature of dislocation pile-up)

$$\beta(x) = \begin{cases} \beta_1(x) & \text{for} \;\; x \in (0, l), \\ \beta_m & \text{for} \;\; x \in (l, a-l), \\ \beta_1(a-x) & \text{for} \;\; x \in (a-l, a), \end{cases}$$

Functional

$$E = 2\int_0^l \left[\frac{1}{2}(\gamma - \beta_1)^2 + k\left(\beta_1' + \frac{1}{2}\beta_1'^2 \right) \right] dx + \frac{1}{2}(\gamma - \beta_m)^2 (a - 2l).$$

Function $\beta_1(x)$ is subject to the boundary conditions

$$\beta_1(0) = 0, \quad \beta_1(l) = \beta_m.$$

Varying this energy functional with respect to $\beta_1(x)$ we obtain the Euler equation for $\beta_1(x)$ on the interval $(0, l)$

$$\gamma - \beta_1 + k\beta_1'' = 0.$$

The variation of energy functional with respect to β_m and l yields the two additional boundary conditions at $x = l$

$$\beta_1'(l) = 0, \quad 2k = (\gamma - \beta_m)(a - 2l).$$

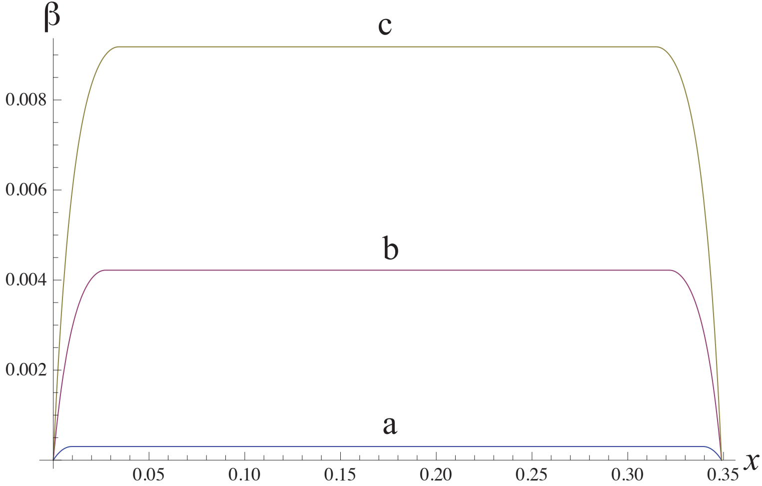
Solution

$$\beta_1(x) = \gamma - \gamma(\cosh \frac{x}{\sqrt{k}} - \tanh \frac{l}{\sqrt{k}} \sinh \frac{x}{\sqrt{k}}), \quad 0 \leq x \leq l.$$

Transcendental equation to determine l

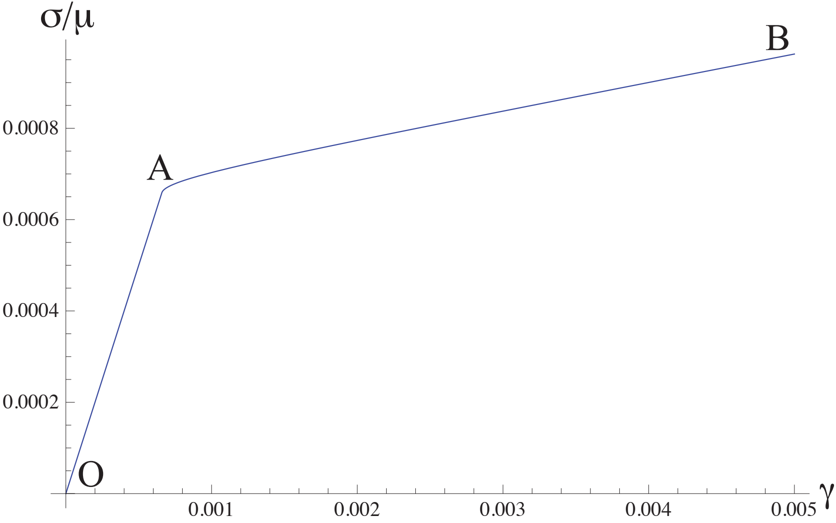
$$f(l) \equiv 2l + 2\frac{k}{\gamma} \cosh \frac{l}{\sqrt{k}} = a.$$

Evolution of plastic distortion



Evolution of β: a)$\gamma = 0.001$, b)$\gamma = 0.005$, c)$\gamma = 0.01$

Stress strain curve



Non-zero dissipation

For the case with dissipation ($\dot{\beta} > 0$) we have to solve the evolution equation

$$\gamma - \beta + k\beta_{,xx} = \gamma_c, \quad \beta(0) = \beta(a) = 0,$$

with $\gamma_c = K/\mu$. Introduce the deviation of $\gamma(t)$ from the critical shear, γ_c, $\gamma_r = \gamma - \gamma_c > 0$

$$\gamma_r - \beta + k\beta'' = 0.$$

Thus, $\beta = \gamma_r \beta_1$. Similarly, for $\dot{\beta} < 0$: in all formulas γ must be replaced by $\gamma_l = \gamma + \gamma_c$. For $\dot{\beta} = 0$ the evolution equation need not be satisfied. It is replaced by $\dot{\beta} = 0$, so the plastic distortion is frozen.

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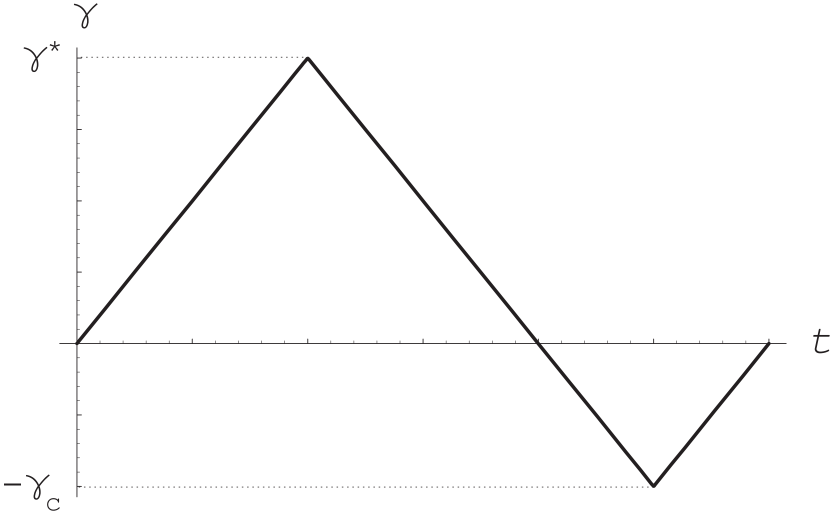

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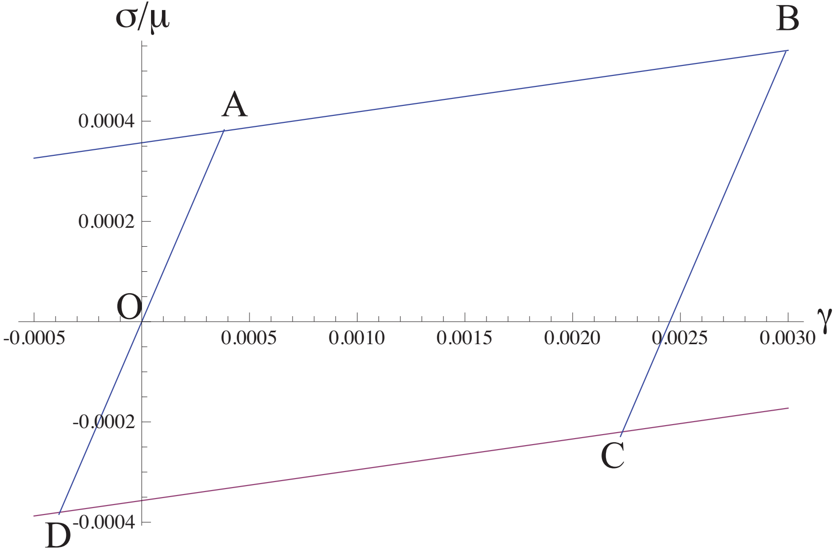
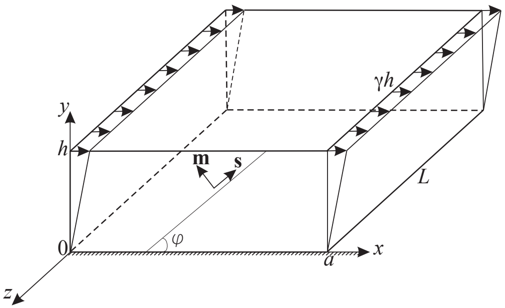
Hysteresis and Bauschinger effect



Average shear stress versus shear strain curve

Plane strain constrained shear



A single crystal strip is placed in a “hard” device with the prescribed displacements at the boundary

$$u = \gamma y, \quad v = 0 \quad \text{at } y = 0, h$$

γ overall shear strain (control parameter)
Assumption: $h \ll a \ll L$

Single slip system

The plastic distortion tensor

$$\beta_{ij} = \beta(y) s_i m_j$$

where

$$\mathbf{s} = (\cos\varphi, \sin\varphi, 0), \quad \mathbf{m} = (-\sin\varphi, \cos\varphi, 0)$$

Since dislocation cannot reach the boundary $y = 0, h$, the plastic distortion $\beta(y)$ satisfies the constraints:

$$\beta(0) = \beta(h) = 0$$

Strain measures

Total strain

$$\varepsilon_{xx} = 0, \quad \varepsilon_{xy} = \frac{1}{2} u_{,y}, \quad \varepsilon_{yy} = v_{,y}$$

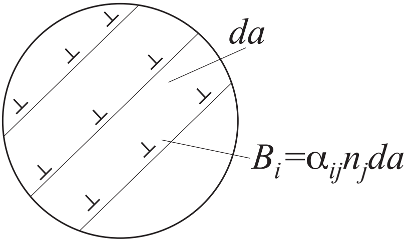
Plastic strains

$$\varepsilon^p_{xx} = -\frac{1}{2}\beta \sin 2\varphi, \quad \varepsilon^p_{xy} = \frac{1}{2}\beta \cos 2\varphi, \quad \varepsilon^p_{yy} = \frac{1}{2}\beta \sin 2\varphi$$

Elastic strain

$$\varepsilon^e_{xx} = \frac{1}{2}\beta \sin 2\varphi, \quad \varepsilon^e_{xy} = \frac{1}{2}(u_{,y} - \beta \cos 2\varphi),$$
$$\varepsilon^e_{yy} = v_{,y} - \frac{1}{2}\beta \sin 2\varphi$$

Nye's dislocation density



Non-zero components of dislocation density tensor

$$\alpha_{xz} = \beta_{,y} \sin\varphi \cos\varphi, \quad \alpha_{yz} = \beta_{,y} \sin^2\varphi$$

Scalar dislocation density

$$\rho = \frac{1}{b}\sqrt{\alpha_{xz}^2 + \alpha_{yz}^2} = \frac{1}{b}|\beta_{,y}||\sin\varphi|$$

Energy density

Energy per unit volume of dislocated crystal

$$\psi(\varepsilon^e_{ij}, \alpha_{ij}) = \frac{1}{2}\lambda\left(\varepsilon^e_{ii}\right)^2 + \mu\varepsilon^e_{ij}\varepsilon^e_{ij} + \mu k \ln \frac{1}{1-\frac{\rho}{\rho_s}}$$

λ, μ - Lamé constants, b - magnitude of Burgers' vector, ρ_s - saturated dislocation density, k - material constant

Energy functional

$$E = aL \int_0^h \Big[\frac{1}{2}\lambda v_{,y}^2 + \frac{1}{2}\mu(u_{,y} - \beta\cos 2\varphi)^2 + \frac{1}{4}\mu\beta^2\sin^2 2\varphi$$
$$+ \mu(v_{,y} - \frac{1}{2}\beta\sin 2\varphi)^2 + \mu k \ln \frac{1}{1 - \frac{|\beta_{,y}||\sin\varphi|}{b\rho_s}} \Big] dy$$

Reduced energy functional

Minimization with respect to u and v leads to

$$E(\beta) = aL \int_0^h \mu \Big[\frac{1}{2}(1-\kappa)\beta^2 \sin^2 2\varphi + \frac{1}{2}\kappa \langle\beta\rangle^2 \sin^2 2\varphi + \frac{1}{2}(\gamma - \langle\beta\rangle \cos 2\varphi)^2 + k \ln \frac{1}{1 - \frac{|\beta_{,y}||\sin\varphi|}{b\rho_s}} \Big] dy$$

where $\langle\beta\rangle = \frac{1}{h}\int_0^h \beta(y)\, dy$

Energy minimization

If the resistance to dislocation motion is negligible, the true plastic distortion minimizes the total energy

Energetic threshold

$$\boxed{\gamma_{en} = \frac{2k}{hb\rho_s}\frac{|\sin\varphi|}{|\cos 2\varphi|}}$$

Size effect: the threshold value is inversely proportional to the size h.

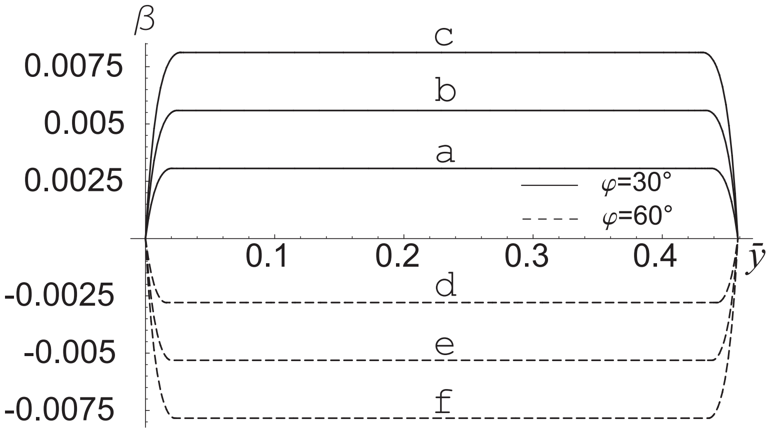
Material parameter

Material	μ (GPa)	ν	b (Å)	ρ_s (μm^{-2})	k
Aluminum	26.3	0.33	2.5	$1.834\,10^3$	0.000156

Table: Material characteristics

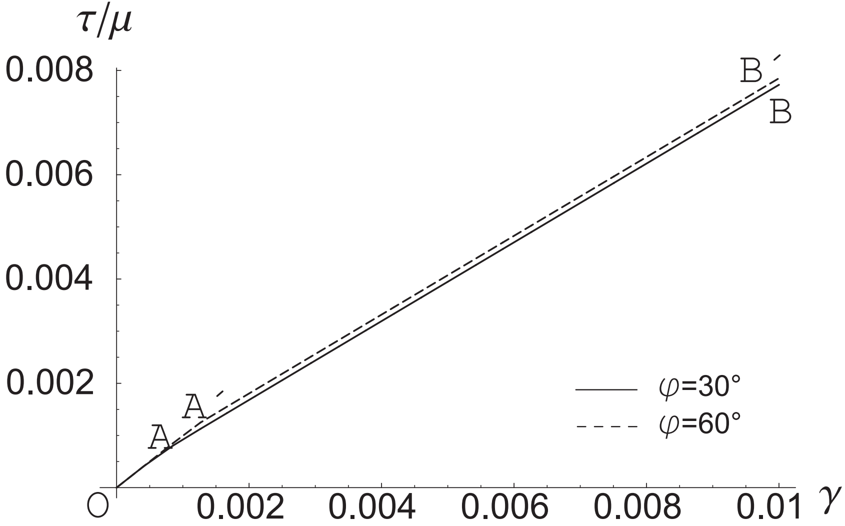
In all simulations $h = 1\mu$m

Evolution of plastic distortion



Evolution of β: a,d)$\gamma = 0.0068$, b,e)$\gamma = 0.0118$, c,f)$\gamma = 0.0168$

Stress strain curve



Non-zero dissipation

Non-zero resistance to dislocation motion: energy minimization is replaced by the flow rule

$$\frac{\partial D}{\partial \dot{\beta}} = -\frac{\delta_\gamma \psi}{\delta \beta}$$

for $\dot{\beta} \neq 0$, where

$$D = K|\dot{\beta}|$$

$$\varkappa \equiv -\frac{\delta_\gamma \psi}{\delta \beta} = -\frac{\partial \psi}{\partial \beta} + \frac{\partial}{\partial y}\frac{\partial \psi}{\partial \beta_{,y}}$$

Plastic distortion may evolve only if the yield condition $|\varkappa| = K$ is fulfilled. If $|\varkappa| < K$, then the plastic distortion β is frozen

Yield condition

Differential equation

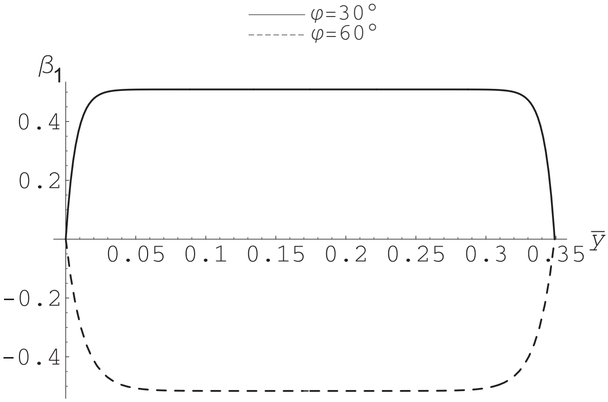
$$|k\frac{\beta_{,yy}\sin^2\varphi}{b^2\rho_s^2}-(1-\kappa)\beta\sin^2 2\varphi$$
$$-(\cos^2 2\varphi+\kappa\sin^2 2\varphi)\langle\beta\rangle+\gamma\cos 2\varphi|=K/\mu=\gamma_{cr}\cos 2\varphi$$

Boundary conditions

$$\beta(0)=\beta(h)=0$$

Evolution of plastic distortion

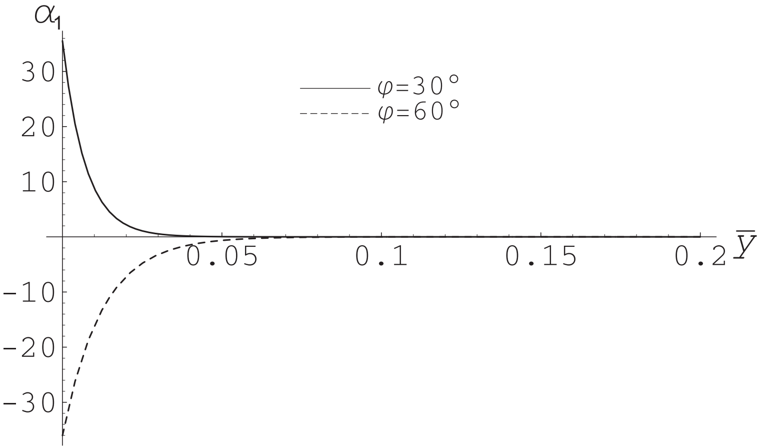
$$\beta(y) = \gamma_r \beta_1(y), \quad \text{where} \quad \gamma_r = \gamma - \gamma_{cr}$$



Graphs of $\beta_1(\bar{y})$

Dislocation density

$\alpha(y) = \gamma_r \alpha_1(y)$



Graphs of $\alpha_1(\bar{y})$

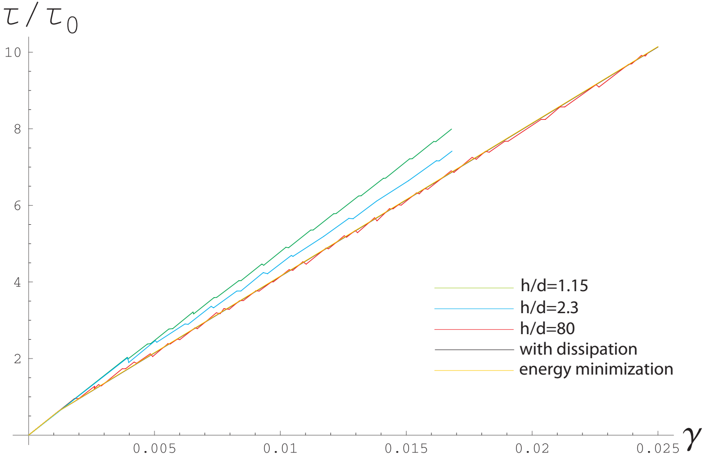
Size effect for hardening rate

It is interesting to calculate the shear stress τ which is a measurable quantity. During the loading, we have for the normalized shear stress

$$\frac{\tau}{\mu} = \gamma_{cr} + \gamma_r \left(1 - \left(1 - \frac{2 \tanh \frac{\eta h}{2}}{\eta h} \right) \beta_{1p} \cos 2\varphi \right)$$

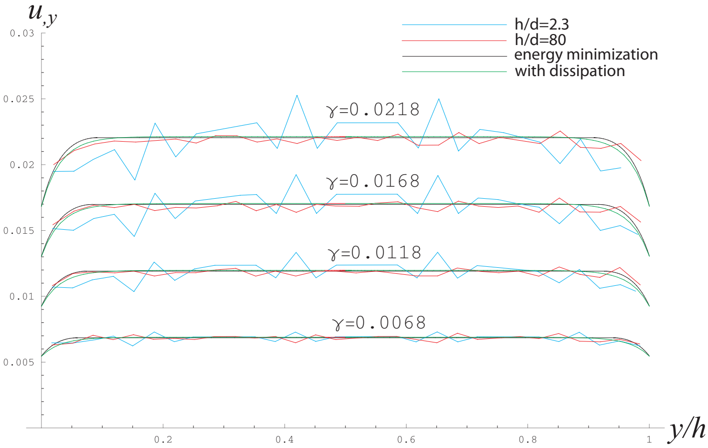
where β_{1p} is calculated from the solution. The second term of this equation causes the hardening due to the dislocations pile-up and describes the size effect in this model.

Comparison



Shear stress vs. shear strain curve

Comparison



Shear strain profile

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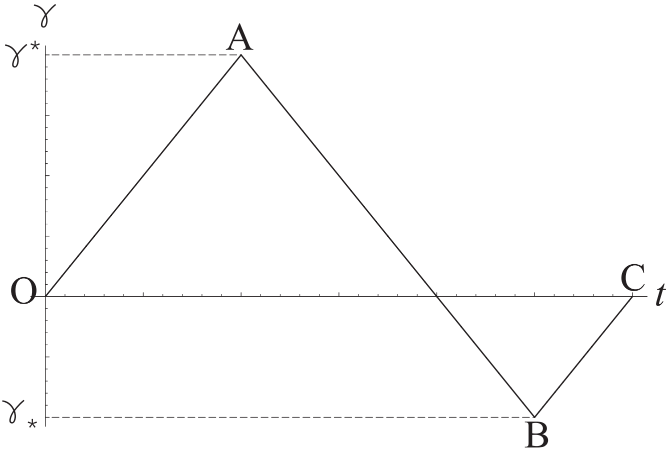

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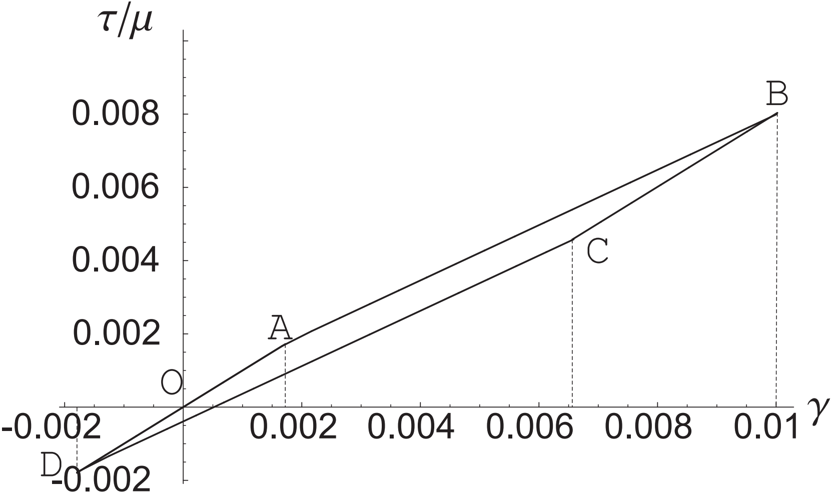
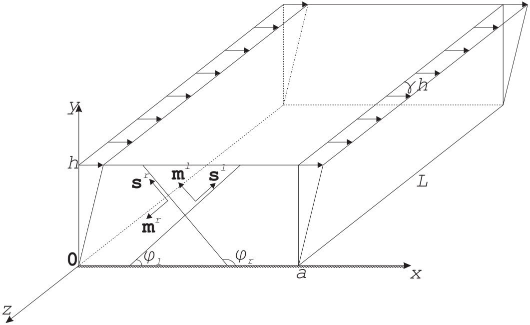
Bauschinger effect



Normalized shear stress versus shear strain curve for $\varphi = 60^\circ$

Double slip system



Tensor of plastic distortion

$$\beta_{ij}(y) = \beta_l(y) s^l_i m^l_j + \beta_r(y) s^r_i m^r_j$$

with $\beta_l(y)$ and $\beta_r(y)$ satisfying

$$\beta_l(0) = \beta_l(h) = \beta_r(0) = \beta_r(h) = 0$$

Strain measures

Total strain

$$\varepsilon_{xx} = 0, \quad \varepsilon_{xy} = \frac{1}{2} u_{,y}, \quad \varepsilon_{yy} = v_{,y}$$

Plastic strains

$$\varepsilon^p_{xx} = -\frac{1}{2}(\beta_l \sin 2\varphi_l + \beta_r \sin 2\varphi_r),$$

$$\varepsilon^p_{xy} = \frac{1}{2}(\beta_l \cos 2\varphi_l + \beta_r \cos 2\varphi_r),$$

$$\varepsilon^p_{yy} = \frac{1}{2}(\beta_l \sin 2\varphi_l + \beta_r \sin 2\varphi_r)$$

Elastic strain

$$\varepsilon^e_{xx} = \frac{1}{2}(\beta_l \sin 2\varphi_l + \beta_r \sin 2\varphi_r),$$

$$\varepsilon^e_{xy} = \frac{1}{2}(u_{,y} - \beta_l \cos 2\varphi_l - \beta_r \cos 2\varphi_r),$$

$$\varepsilon^e_{yy} = v_{,y} - \frac{1}{2}(\beta_l \sin 2\varphi_l + \beta_r \sin 2\varphi_r)$$

Nye's dislocation density

Non-zero components of Nye's dislocation density tensor

$$\alpha_{xz} = \beta_{l,y} \sin\varphi_l \cos\varphi_l + \beta_{r,y} \sin\varphi_r \cos\varphi_r$$
$$\alpha_{yz} = \beta_{l,y} \sin^2\varphi_l + \beta_{r,y} \sin^2\varphi_r$$

Scalar dislocation density

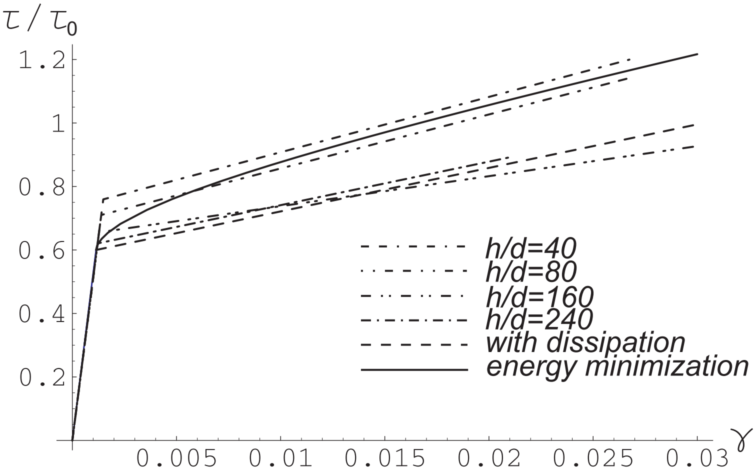
$$\rho = \rho_l + \rho_r$$
$$= \frac{1}{b}|\beta_{l,y} \sin\varphi_l| + \frac{1}{b}|\beta_{r,y} \sin\varphi_r|$$

Energetic threshold

$$\gamma_{en} = \frac{2k}{hb\rho_s} \frac{|\sin\varphi|}{|\cos 2\varphi|}$$

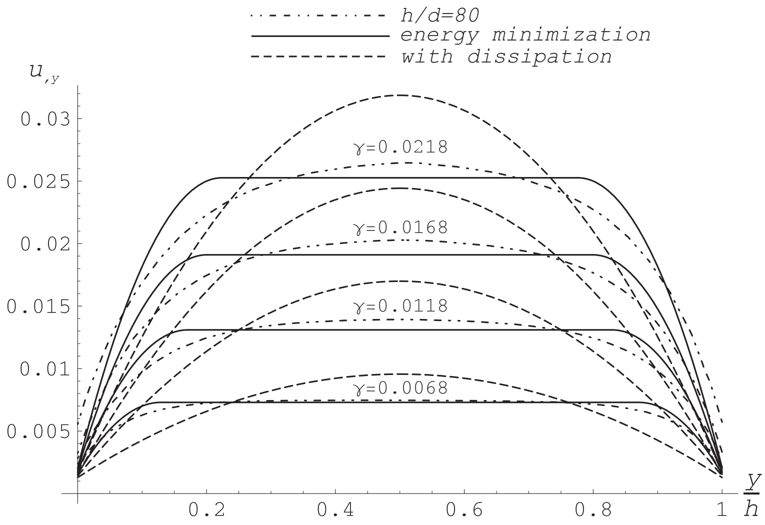
Size effect: the threshold value is inversely proportional to the size h. Mention that the energetic threshold value for the symmetric double slip is equal to that of the single slip found in (Le & Sembiring, 2007).

Comparison



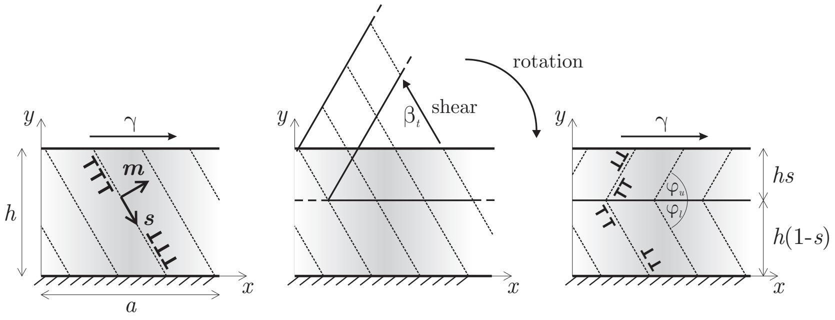
Shear stress vs. shear strain curve

Comparison



The total shear strain profiles

Mechanism of twins formation



The twin phase is formed by a twinning shear produced by the movement of pre-existing dislocations to the boundary followed by a rigid rotation. The described mechanism of twin formation is closely related to that of Bullough (1957). The difference is that dislocations need not to glide through each lattice plane.

Continuum model of deformation twinning

Tensor of plastic distortion

$$\beta_{ij}(y) = \begin{cases} \beta s_i^l m_j^l & \text{for } 0 < y < h(1-s), \\ \beta s_i^u m_j^u + \beta_t s_i^l m_j^l + \omega_{ij} & \text{for } h(1-s) < y < h, \end{cases}$$

with $\beta(y)$ satisfying the constraints:

$$\beta(0) = \beta(h) = \beta\left(h(1-s)\right) = 0$$

The twinning shear is given by $\beta_t = -2\cot\varphi$

Plastic strains

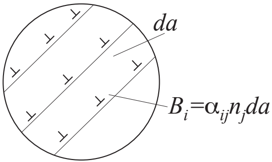
The in-plane components of the plastic strain tensor $\varepsilon^p_{ij} = \frac{1}{2}(\beta_{ij} + \beta_{ji})$ read

$$\varepsilon^p_{xx} = -\frac{1}{2}\beta \sin 2\varphi - \frac{1}{2}\beta_T \sin 2\varphi_l,$$
$$\varepsilon^p_{xy} = \frac{1}{2}\beta \cos 2\varphi + \frac{1}{2}\beta_T \cos 2\varphi_l,$$
$$\varepsilon^p_{yy} = \frac{1}{2}\beta \sin 2\varphi + \frac{1}{2}\beta_T \sin 2\varphi_l,$$

with the following quantities defined in the upper and lower part of the crystal:

$$[\beta(y),\ \varphi,\ \beta_T] = \begin{cases} [\beta_u(y),\ \varphi_u,\ \beta_t] & h(1-s) < y < h, \\ [\beta_l(y),\ \varphi_l,\ 0] & 0 < y < h(1-s). \end{cases}$$

Dislocation density



Non-zero components of dislocation density tensor

$$\alpha_{xz} = \beta_{,y} \sin\varphi \cos\varphi, \quad \alpha_{yz} = \beta_{,y} \sin^2\varphi$$

Scalar dislocation density

$$\rho = \frac{1}{b}\sqrt{\alpha_{xz}^2 + \alpha_{yz}^2} = \frac{1}{b}|\beta_{,y}||\sin\varphi|$$

Energy density

Free energy per unit volume of dislocated crystal

$$\psi(\varepsilon^e_{ij}, \alpha_{ij}) = \frac{1}{2}\lambda\left(\varepsilon^e_{ii}\right)^2 + \mu\varepsilon^e_{ij}\varepsilon^e_{ij} + \mu k \ln \frac{1}{1 - \frac{\rho}{\rho_s}}$$

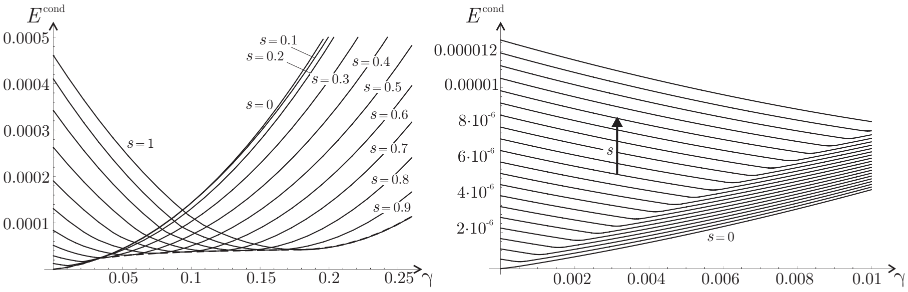
λ, μ - Lamé constants, b - magnitude of Burgers' vector, ρ_s - saturated dislocation density, k - material constant

Energy functional

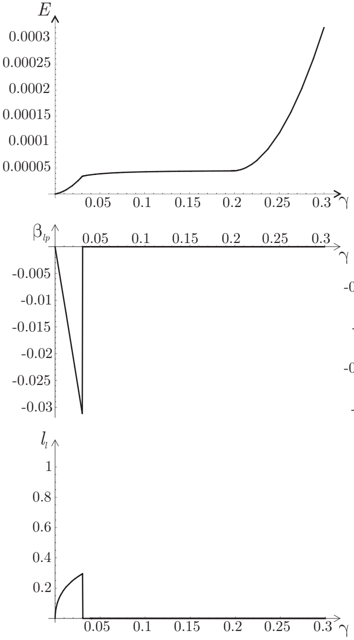
$$
\begin{aligned}
E(u,v,\beta,s) = aL\int_0^h \Big[& \tfrac{1}{2}\lambda v_{,y}^2 + \tfrac{1}{4}\mu(\beta\sin 2\varphi + \beta_T \sin 2\varphi_I)^2 \\
& + \tfrac{1}{2}\mu(u_{,y} - \beta\cos 2\varphi - \beta_T\cos 2\varphi_I)^2 \\
& + \mu(v_{,y} - \tfrac{1}{2}\beta\sin 2\varphi - \tfrac{1}{2}\beta_T\sin 2\varphi_I)^2 \\
& + \mu k \ln \frac{1}{1 - \frac{|\beta_{,y}\sin\varphi|}{b\rho_s}} \Big]\, dy.
\end{aligned}
$$

TWIP-alloys have rather low stacking fault energies, so the contribution of surface energy to this functional can be neglected.

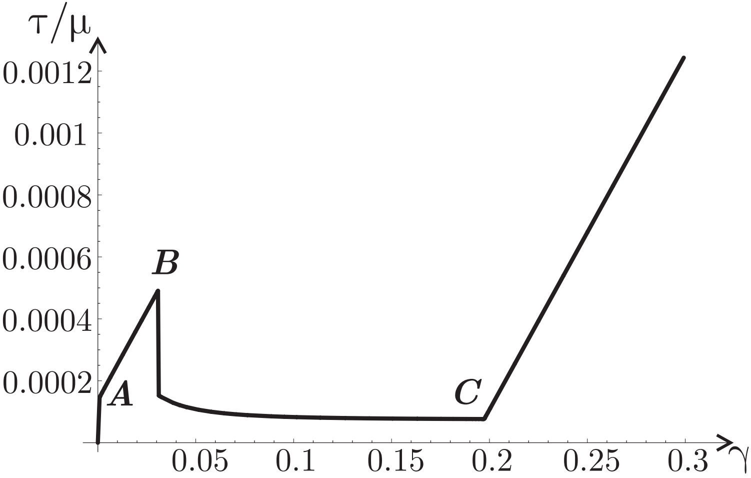
Condensed energy



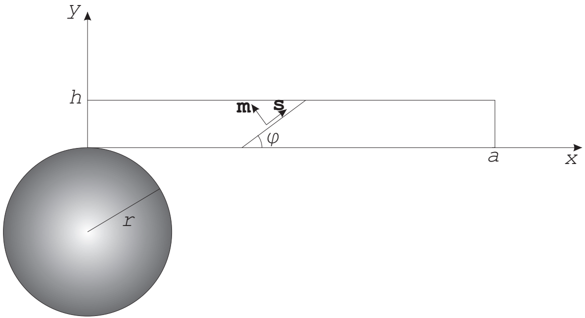
Condensed energy $E^{\text{cond}}(s,\gamma) = \min_\beta E(\beta, s, \gamma)$ versus overall shear strain γ for various volume fractions s (left) with a magnification (right) for small values of s and small strains (clearly indicating that $s = 0$ minimizes the energy in that region). The actual energy with evolving s follows the path of least energy


E
0.0003
0.00025
0.0002
0.00015
0.0001
0.00005
0.05 0.1 0.15 0.2 0.25 0.3 γ
s
1
0.8
0.6
0.4
0.2
0.05 0.1 0.15 0.2 0.25 0.3 γ
β_{lp}
0.05 0.1 0.15 0.2 0.25 0.3 γ
-0.005
-0.01
-0.015
-0.02
-0.025
-0.03
β_{up}
0.05 0.1 0.15 0.2 0.25 0.3 γ
-0.05
-0.1
-0.15
-0.2
l_l
1
0.8
0.6
0.4
0.2
0.05 0.1 0.15 0.2 0.25 0.3 γ
l_u
0.5
0.4
0.3
0.2
0.1
0.05 0.1 0.15 0.2 0.25 0.3 γ

Stress-strain curve



Bending



A single crystal beam is bent along a rigid cylinder. The displacements of the lower face are prescribed

$$u_x(x,0) = r\sin(x/r) - x, \quad u_y(x,0) = r\cos(x/r) - r$$

Assumption: $h \ll a$

Single slip system

Tensor of plastic distortion

$$\beta_{ij} = \beta(x, y) s_i m_j, \ \mathbf{s} = (\cos\varphi, \sin\varphi), \ \mathbf{m} = (-\sin\varphi, \cos\varphi)$$

Plastic strains

$$\varepsilon^p_{xx} = -\frac{1}{2}\beta \sin 2\varphi, \ \varepsilon^p_{yy} = \frac{1}{2}\beta \sin 2\varphi, \ \varepsilon^p_{xy} = \frac{1}{2}\beta \cos 2\varphi$$

Dislocation density

$$\alpha_{xz} = \beta_{,x} \cos^2\varphi + \beta_{,y} \cos\varphi \sin\varphi,$$
$$\alpha_{yz} = \beta_{,x} \cos\varphi \sin\varphi + \beta_{,y} \sin^2\varphi$$

Scalar dislocation density

$$\rho = \frac{1}{b}\sqrt{(\alpha_{xz})^2 + (\alpha_{yz})^2} = \frac{1}{b}|\beta_{,x} \cos\varphi + \beta_{,y} \sin\varphi|$$

Energy density

Free energy per unit volume of dislocated crystal

$$\psi(\varepsilon^e_{ij}, \alpha_{ij}) = \frac{1}{2}\lambda\left(\varepsilon^e_{ii}\right)^2 + \mu\varepsilon^e_{ij}\varepsilon^e_{ij} + \mu k \ln \frac{1}{1 - \frac{\rho}{\rho_s}}$$

λ, μ - Lamé constants, b - magnitude of Burgers' vector, ρ_s - saturated dislocation density, k - material constant

Energy functional of the bent beam

$$I = \int_0^a \int_0^h [\frac{1}{2}\lambda(u_{x,x} + u_{y,y})^2 + \mu(u_{x,x} + \frac{1}{2}\beta \sin 2\varphi)^2 + \mu(u_{y,y} - \frac{1}{2}\beta \sin 2\varphi)^2 + \frac{1}{2}\mu(u_{x,y} + u_{y,x} - \beta \cos 2\varphi)^2 + \mu k \ln \frac{1}{1 - \frac{|\beta_{,x}\cos\varphi + \beta_{,y}\sin\varphi|}{b\rho_s}}]\, dxdy$$

Because of the prescribed displacements at $y = 0$ dislocations cannot reach the lower face of the beam which is in contact with the bending jig in the deformed state, therefore

$$\beta(x, 0) = 0$$

Reduced energy functional

Variational-asymptotic analysis reduces the energy functional containing the small parameter h/a to

$$E_1 = \int_0^a \int_0^h [\kappa(\cos\frac{x}{r} - 1 + \frac{1}{2}\beta' \sin 2\varphi)^2 + k|\beta'_{,y} \sin\varphi| + \frac{1}{2}k(\beta'_{,y} \sin\varphi)^2]\, dxdy$$

where κ is given by

$$\kappa = \frac{1}{1-\nu},$$

Energy minimization

In the equilibrium state the true plastic distortion minimizes the total energy

Smooth minimizer

The plastic distortion

$$\beta'(x,y) = \begin{cases} \beta_1(x,y) & \text{for } y \in (0, l(x)), \\ \beta_0(x) & \text{for } y \in (l(x), h) \end{cases}$$

where

$$\beta_1(x,y) = \beta_{1p}(1 - \cosh \chi y + \tanh \chi l(x) \sinh \chi y)$$

$$\beta_{1p} = -\frac{2}{\sin 2\varphi}(\cos \frac{x}{r} - 1), \quad \chi = \sqrt{\frac{2\kappa}{k}} \cos \varphi$$

Transcendental equation to determine $l(x)$

$$k \sin \varphi + \kappa[(\cos \frac{x}{r} - 1)$$
$$+ \frac{1}{2}\beta_{1p}(1 - \frac{1}{\cosh \chi l(x)})] \sin 2\varphi) \sin 2\varphi(h - l(x)) = 0.$$

Energetic threshold

Size effect: the threshold value depends on a and h

$$\boxed{r_{cr} = \frac{a}{\arccos(1 - \frac{k}{2\kappa h \cos\varphi})}}$$

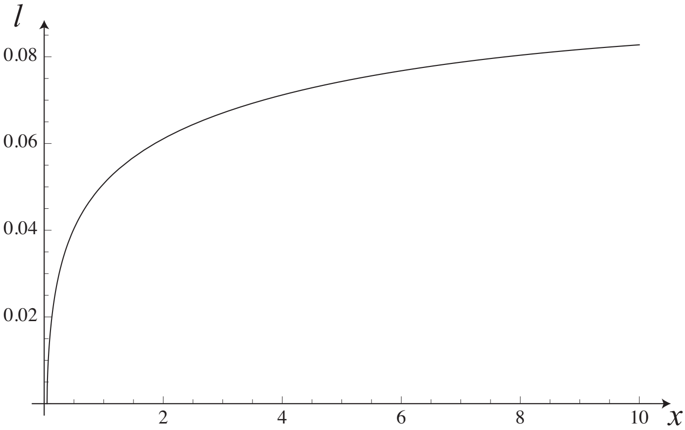
Thus, if the radius of the bending jig $r > r_{cr}$, then $l(x) = 0$ and $\beta = 0$ everywhere yielding the purely elastic deformation without dislocations. For $r < r_{cr}$ the dislocations are nucleated and pile-up against the lower boundary $y = 0$ with $x > x_*$ forming there the boundary layer.

Material parameter

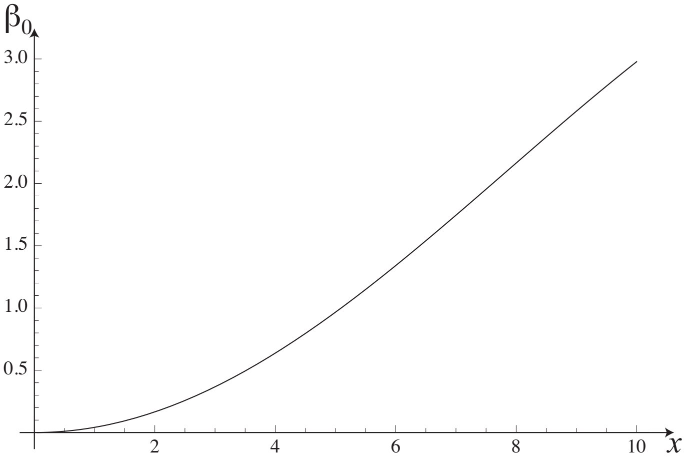
Material	μ (GPa)	ν	b (Å)	ρ_s (μm^{-2})	k
Zinc	43	0.25	2.68	145.4	0.000156

Table: Material characteristics

In all simulations $a = 10$mm, $h = 1.3$mm, $\varphi = 35^\circ$.

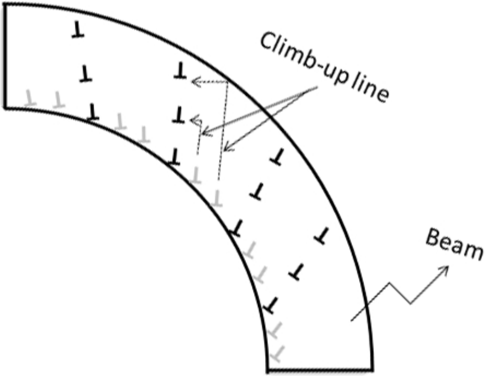


Function $l(x)$.



Function $\beta_0(x)$.

Polygonization



During annealing dislocations may climb in the transversal direction and then glide along the slip direction and be rearranged as shown in this Figure.

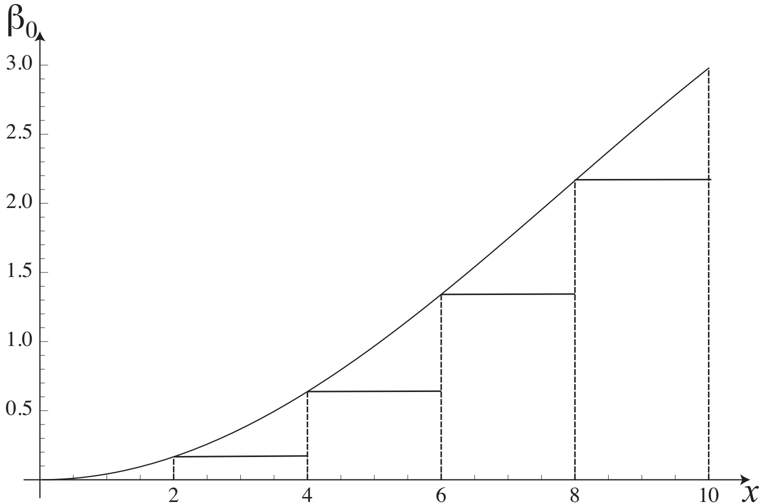
After annealing

In the final polygonized relaxed state the dislocations form low angle tilt boundaries between polygons which are perpendicular to the slip direction, while inside the polygons there are no dislocations. We want to show that this rearrangement of dislocations correspond to a sequence of piecewise constant $\check{\beta}(x,y)$ reducing energy of the beam. Here and below check is used to denote the polygonized relaxed state after annealing. The jump of $\check{\beta}$ means the dislocations concentrated at the surface, therefore we ascribe to each jump point the normalized Read-Shockley surface energy density

$$\gamma([\![\check{\beta}]\!]) = \gamma_* |[\![\check{\beta}]\!]| \ln \frac{e\beta_*}{|[\![\check{\beta}]\!]|},$$

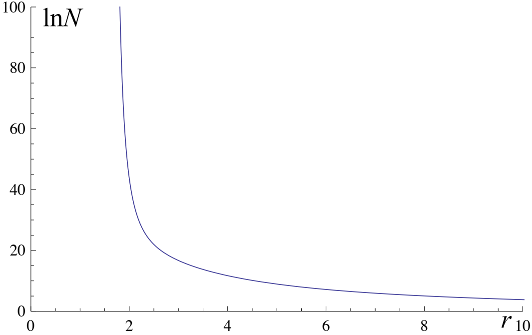
with $[\![\check{\beta}]\!](x_i) = \check{\beta}(x_i+0) - \check{\beta}(x_i-0)$ denoting the jump of $\check{\beta}(x)$, $\gamma_* = \frac{b}{4\pi(1-\nu)}$, and β_* the saturated misorientation angle.

Energy reducing sequence



Number of polygons

The number of polygons can be estimated from above by requiring that the increase of the surface energy is less than the reduction of the bulk energy in gradient terms. For the material parameters of zinc, the estimated average polygon distance (taken as the length of the beam divided by the number of polygons) is equal to around 2.7×10^{-7} m which is in excellent agreement with the experimental result obtained by Gilman in 1955.



Conclusions

- CDT enables ones to model dislocation pile-up and size effects
- There exists a threshold value for the dislocation nucleation depending on the grain size
- Work hardening and Bauschinger effect can properly be described
- Deformation twins exhibit another type of non-convexity
- Existence of distinct thresholds for the onset of deformation twinning
- The stress-strain response exhibits a sharp load drop (followed by a stress plateau) upon the onset of twinning
- Polygonization occurs due to the smallness of the Read-Shockley surface energy as compared with the bulk energy of distributed dislocations
- The rearrangement of dislocations is realized by the dislocation climb with the subsequent dislocation glide.
- High-temperature dislocation climb during annealing is crucial for the kinetics of polygonization

Further works

- Indentation
- Bending and torsion
- Particle strengthening
- Multiple slip
- CDT for polycrystals
- Hall-Petch relation
- Plastic zone near the crack tip and ductile fracture
- Finite twinning shear and finite rotation
- Parameter identification and applications to TWIP-alloys
- 3-D model
- Dislocation climb taking into account the interaction with vacancies
- Kinetics of polygonization
- Formation of dislocation cell structure