Crystal plasticity treated as quasi-static material flow trough adjustable crystal lattice

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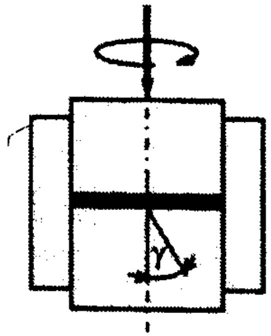
Outline

- Motivation: observed SPD substructures (high pressure torsion)
- Flow model of crystal plasticity
- Example: high pressure torsion

Motivation

high pressure torsion



- After an initial adjustment to a tool, specimens twisted under high axial compression do not change their shape and they withstand unlimited amount of plastic deformation

- An initial non-steady material flow (up to strain >~ 20) is followed by a steady flow (saturation) where no further work hardening and structural changes are observed

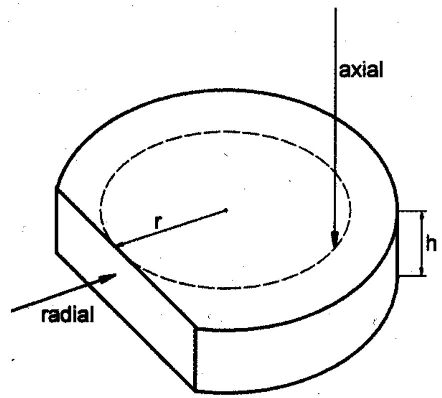
- The observations excluded grain boundary sliding as the main mechanism in explored HPT; the deformation was achieved by intergranular glide

- Strain can be defined approximately as simple shear

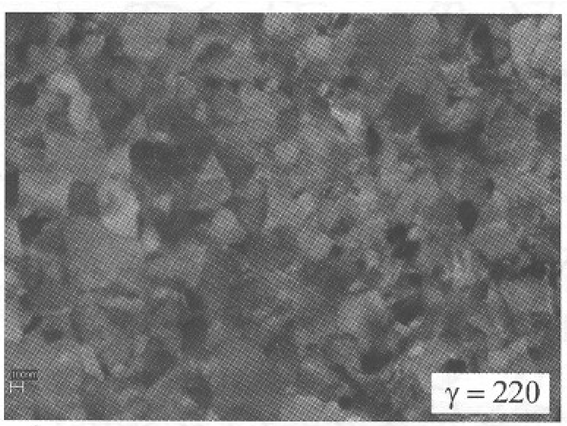
Austrian school: Habesberger, Pippan, Schafler, Stüve, Vorhauer, Wetscher, Zehetbauer

Motivation

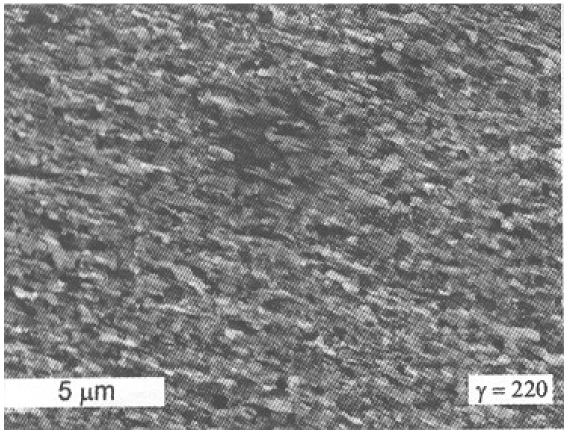
• preferred alignment of structural elements in radial direction inclined with respect to the torsion axis the alignment is changing with reverse of twist no alignment is observed in axial direction



HPT copper: Hebesberger et al.: *Acta Mat.* (2004)



axial viewpoint



radial viewpoint

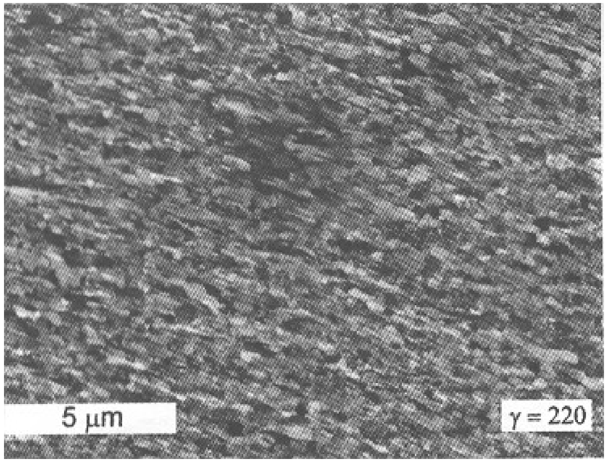
Motivation

Motivated by severe plastic deformation experiments it seems that crystalline materials at yield behave as a special kind of incompressible, anisotropic, highly viscous fluids.

Crystal plasticity can be interpreted as:

material flow though adjustable crystal lattice space

analogously as a riverbed adjusts to a water flow.

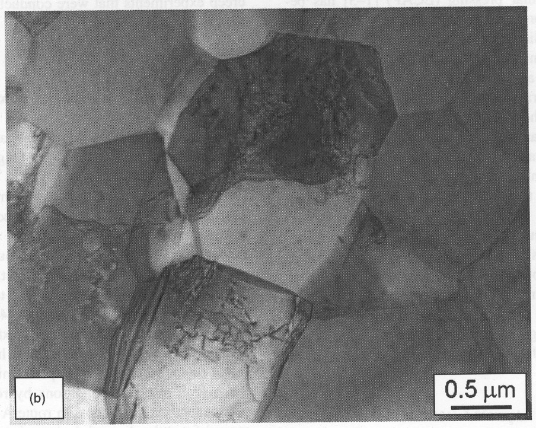


HPT copper: Hebesberger et al.: *Acta Mat.* (2004)

The material flow through the crystal lattice has been regarded by Asaro as crystal plasticity "basic tenet" *Advances in Applied Mechanics,* 1983.

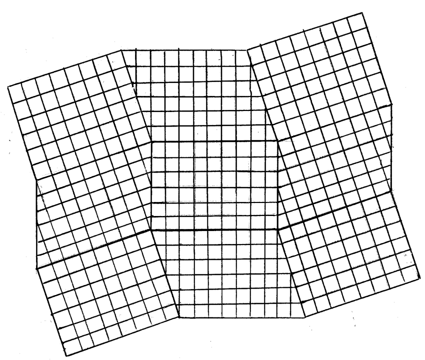
Flow model of crystal plasticity

misoriented cells (subgrains):



TEM micrographs of aluminium after four subsequent ECAP steps on route (a) A and (b) B.

scheme of corresponding lattice space:



crystal plasticity framework:

rate dependent (rigid-viscous-plastic)

principal variables of the model:

$\vec{v}(\vec{x},t)$	velocity
$\nu^{(i)}(\vec{x},t)$	slip rates
$\boldsymbol{R}(\vec{x},t)$	rotation of lattice
$\boldsymbol{T}(\vec{x},t)$	stress
$\tau_{\mathrm{y}}^{(i)}(\vec{x},t)$	yield stresses

$$i = 1, 2, \ldots, I$$

governing equations:

kinematics:
- flow rule
- GND density

dynamics:
- stress equilibrium
- dissipation inequality

constitutive relations:
- yield condition
- hardening law

Flow model of crystal plasticity

Kinematics

$$\boldsymbol{F} = \boldsymbol{F}^{\mathrm{e}}\boldsymbol{F}^{\mathrm{p}}$$

- flow rule:

rate of lattice adjustment — material flow

$$\boldsymbol{L} = \nabla \boldsymbol{v} = \dot{\boldsymbol{R}}\boldsymbol{R}^{\mathrm{T}} + \sum_{i=1}^{I} \nu^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)}$$

$$\boldsymbol{s}^{(i)} = \boldsymbol{R}\boldsymbol{s}_0^{(i)}, \quad \boldsymbol{m}^{(i)} = \boldsymbol{R}\boldsymbol{m}_0^{(i)}$$

material stretching:

$$\boldsymbol{D} = (\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^{\mathrm{T}})/2 = \sum_{i=1}^{I} \nu^{(i)} (\boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)} + \boldsymbol{m}^{(i)} \otimes \boldsymbol{s}^{(i)})/2$$

evolution of lattice adjustment:

$$\dot{\boldsymbol{R}} = [(\nabla \boldsymbol{v} - \nabla \boldsymbol{v}^{\mathrm{T}})/2 - \sum_{i=1}^{I} \nu^{(i)} (\boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)} - \boldsymbol{m}^{(i)} \otimes \boldsymbol{s}^{(i)})/2]\boldsymbol{R}$$

- GND density:

seen in micrographs

$$\boldsymbol{\Lambda} = [\mathrm{curl}\, \boldsymbol{R}^{\mathrm{T}}]\boldsymbol{R}^{\mathrm{T}}$$

Flow model of crystal plasticity

Dynamics

- stress equilibrium: $$\operatorname{div}\boldsymbol{T} = 0$$

- resolved shear stress: $$\tau^{(i)} = \boldsymbol{s}^{(i)} \cdot \boldsymbol{T}\boldsymbol{m}^{(i)}$$

- dissipation inequality: $$\boldsymbol{T} \cdot \boldsymbol{D} = \sum_{i=1}^{I} \tau^{(i)} \nu^{(i)} \geq 0$$

Flow model of crystal plasticity

Constitutive relations

- yield condition: $$\nu^{(i)} = |\frac{\tau^{(i)}}{\tau_y^{(i)}}|^{1/r} \mathrm{sign}\, \tau^{(i)}$$

- hardening law:

$$\dot{\tau}_{\mathrm{y}}^{(i)} = \sum_{j=1}^{I} H_{ij}\, |\nu^{(j)}| + \sum_{j=1}^{I} K_{ij}\, (s^{(i)} \cdot \nabla)(s^{(j)} \cdot \nabla)\nu^{(j)}\,;$$

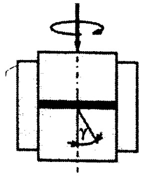
local hardening

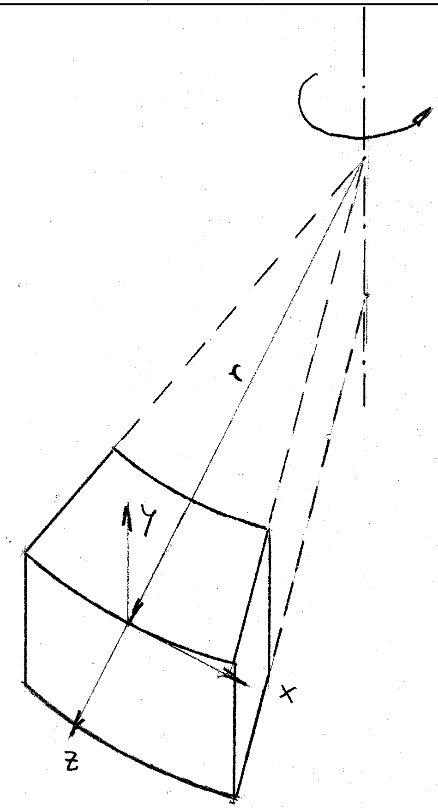
non-local hardening
(close range dislocation interaction)
Grama et al *Acta Materialia* 2003,
Kratochvil et al *Physical Review* 2007

Boundary conditions:
- periodic
- surface layer

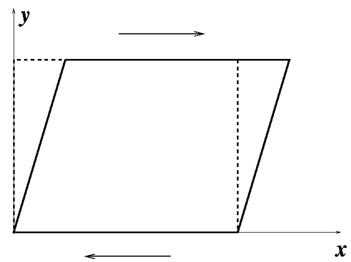
Kuroda & Tvergaard *Int. J. Mechanics and Physics of Solids* 2008

Example: high pressure torsion





radial direction ~ simple shear



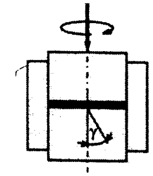
$$\gamma = \frac{r\theta}{h}$$

axial direction ~ plastic strain gradient

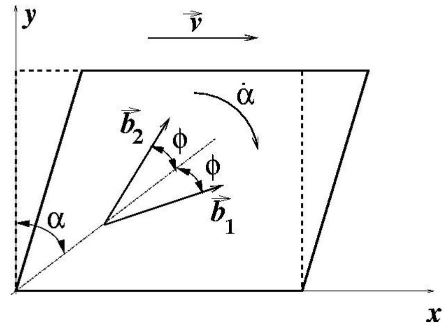
$$\nabla\gamma = \frac{\theta}{h} = b\rho_G\,,\quad \rho_G = \frac{\gamma}{rb}$$

$$\rho_G = 10^{13} - 10^{14}\ \mathrm{m}^{-2}$$

Example: high pressure torsion



double slip rigid-plastic model



v velocity field

α lattice rotation

$\kappa^{(1)}$, $\kappa^{(2)}$ slip rates

rate of lattice rotation material flow

$$\nabla v = \dot{R}R^{-1} + \sum_{i=1}^{2} \kappa^{(i)} s^{(i)} \otimes m^{(i)}$$

in components:

$$\kappa^{(1)} = -\frac{2\frac{\partial v_x}{\partial x}\cos 2(\alpha-\phi) - (\frac{\partial v_x}{\partial y} - \frac{\partial v_y}{\partial x})\sin 2(\alpha-\phi)}{\sin 4\phi} \qquad \kappa^{(2)} = \frac{-2\frac{\partial v_x}{\partial x}\cos 2(\alpha+\phi) + (\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x})\sin 2(\alpha+\phi)}{\sin 4\phi}$$

$$\dot{\alpha} = -\frac{\frac{\partial v_x}{\partial x}\sin 2\alpha + \frac{\partial v_x}{\partial y}\cos(\alpha+\phi)\cos(\alpha-\phi) - \frac{\partial v_y}{\partial x}\sin(\alpha+\phi)\sin(\alpha-\phi)}{\cos 2\phi}$$

Kratochvíl, Kružík and Sedláček: *Acta Materialia* (2009)

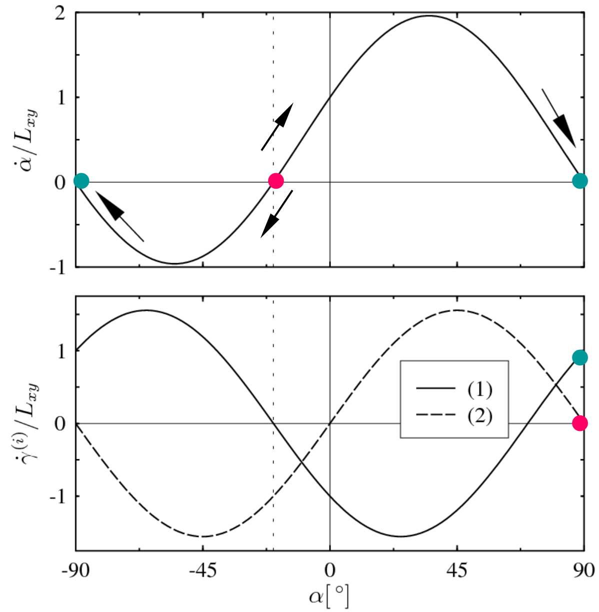
1. rotation of slip systems: homogeneous solution

Kratochvíl, Kružík and Sedláček: *Acta Materialia* (2009)

rate of rotation

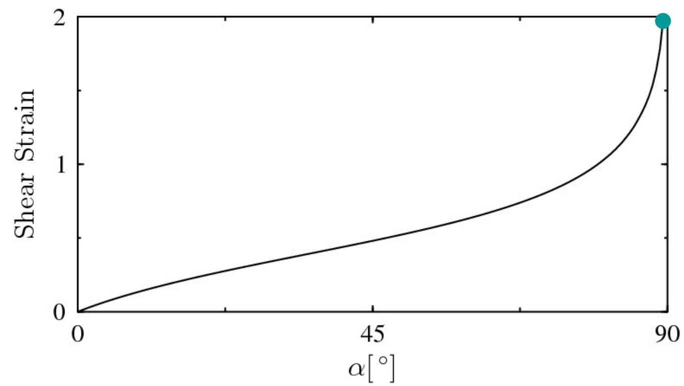
$$L_{xy} = \frac{\partial v_x}{\partial y}$$

double slip activity



steady state single slip

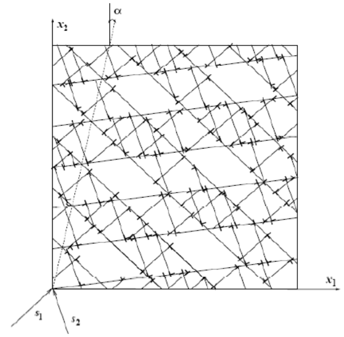
steady state single slip
is reached asymptotically
(saturation)



! homogenous states are unstable !

2. fragmentation = spontaneous structuralization

formation and reconstruction of structural elements (subgrains)



Kratochvíl, Kružík and Sedláček: Rev.Adv.Mater.Sci. (2010)

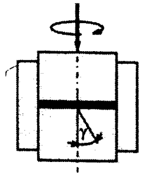
Scheme of misoriented fragmented structural elements.

- fragmentation of crystal or polycrystalline grains into a pattern of structural elements (misoriented cells) is a result of a trend to reduce energetically costly multislip.
- orientation of the pattern follows the orientation of the slip systems

⇓

rotation of the slip systems causes a permanent subgrains reconstruction

Example: high pressure torsion



cell size:

$$R = \frac{4|\tilde{h}|}{\delta h} \approx \frac{2G}{\pi(1-\nu)} \frac{D}{\delta \rho h}$$

Kratochvíl, Kružík and Sedláček: *Phys. Rev. B* (2007)

shear modulus G
hardening h G/h = 100
dislocation density in boundaries $\rho = 10^{16}\ \mathrm{m}^{-2}$
width of non-equilibrium boundaries δ = 10 nm

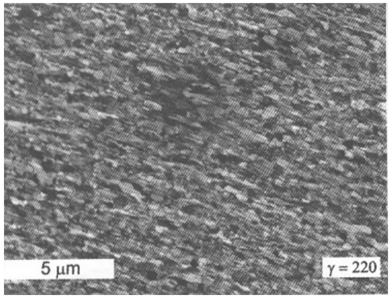
⇒ $R \sim 1\mu\mathrm{m}$

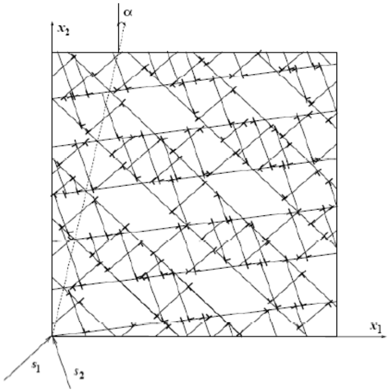
Summary: interpretation of HPT observations

Kratochvíl, Kružík and Sedláček: *Acta Materialia* (2009), Rev.Adv.Mater.Sci. (2010)

key assumption: *glide is carried by a double slip along rotating slip systems*

modeling: material flow through adjustable crystal lattice





observations	model
preferred alignment	√
structural misorientation "3D meanders"	√
saturation	√
size	?