Why does a crystal rotate ?

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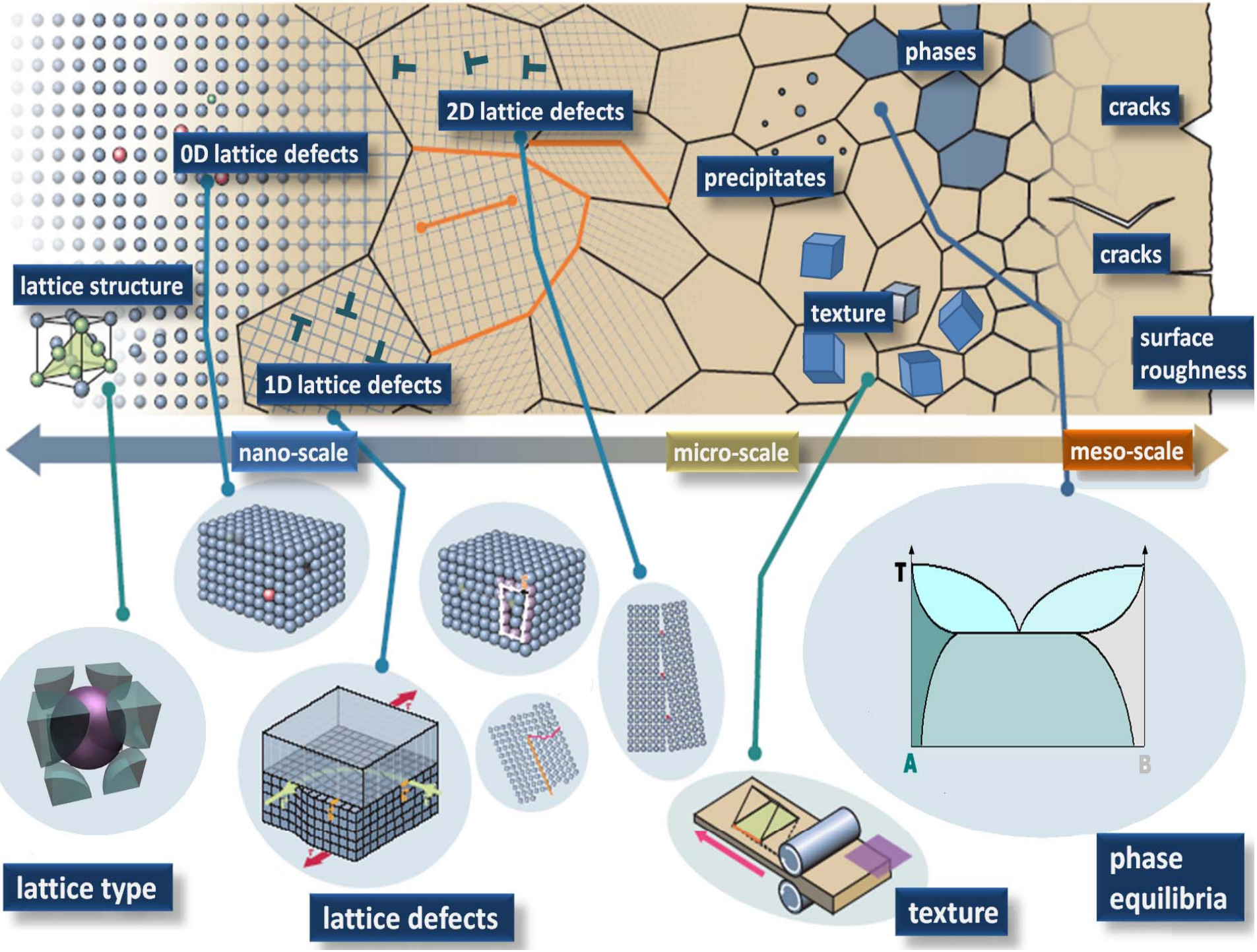
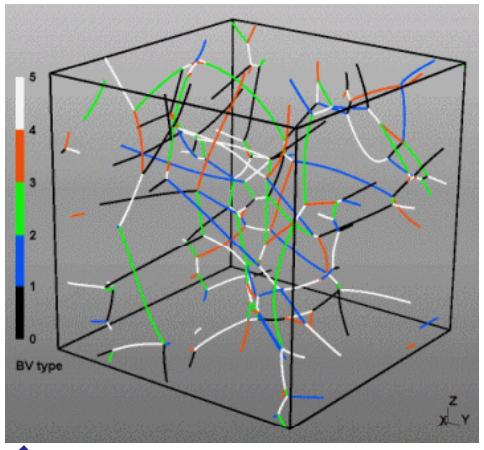
SFB Class 2012

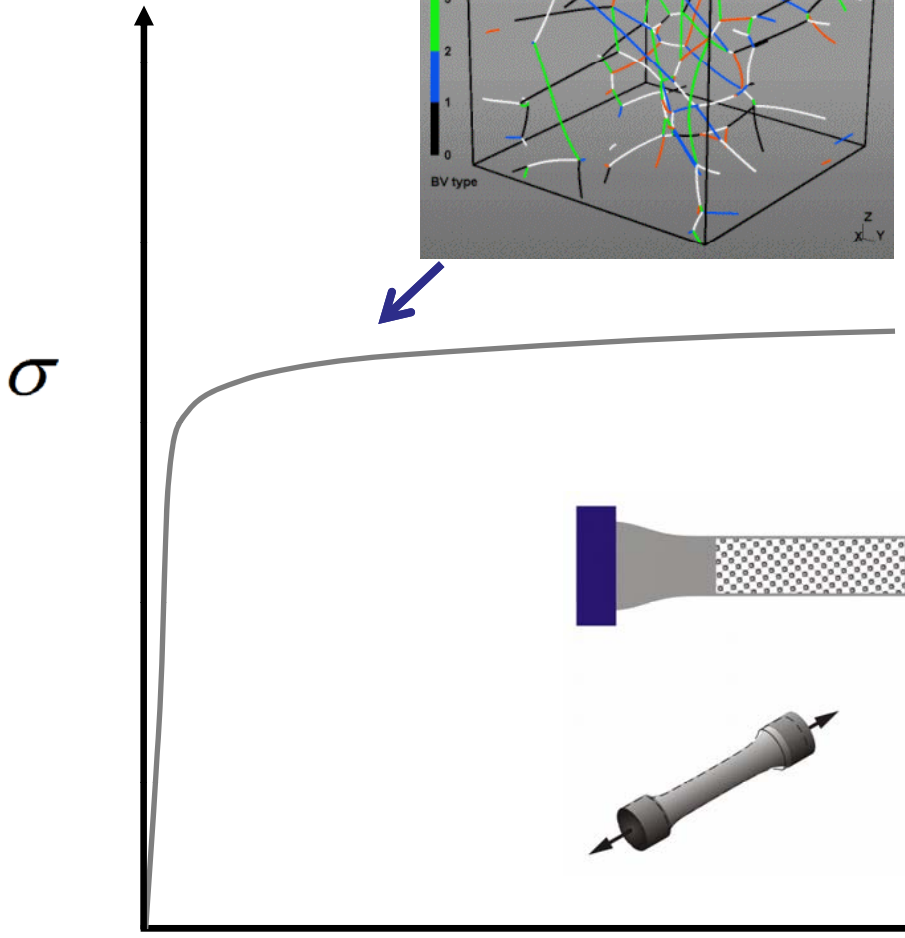
Overview

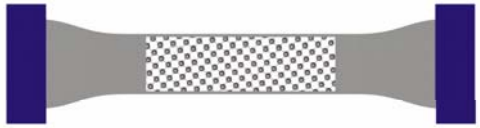
- Rotation of a single crystal
- Single crystal yield surface
- Taylor model for polycrystals
- The Crystal Plasticity Finite Element Method

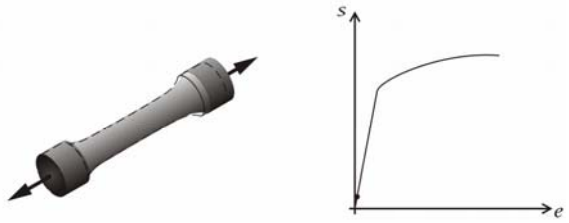

phases
cracks
2D lattice defects
0D lattice defects
precipitates
cracks
lattice structure
texture
surface roughness
1D lattice defects
nano-scale
micro-scale
meso-scale
T
A
B
lattice type
lattice defects
texture
phase equilibria

Some dislocation kinematics and kinetics: phenomena





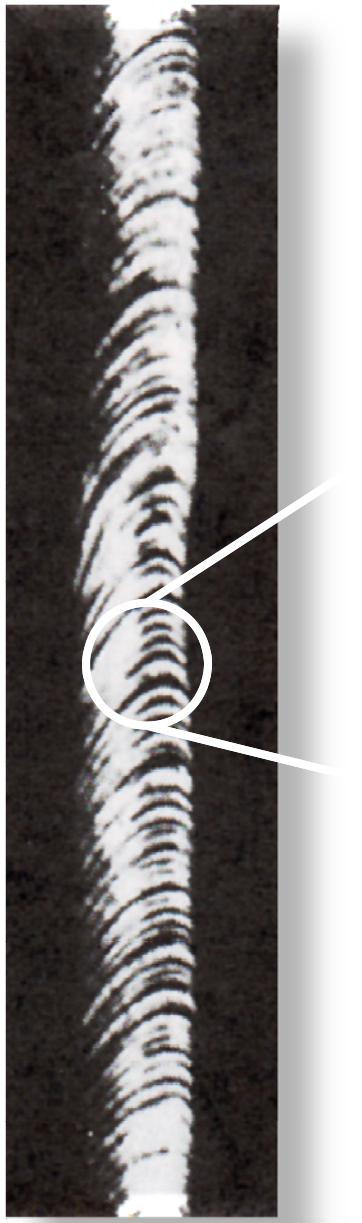


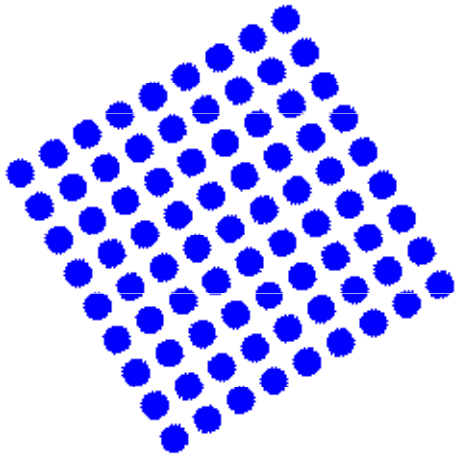


ε true strain

σ stress

Plastic deformation of a single crystal by dislocation slip





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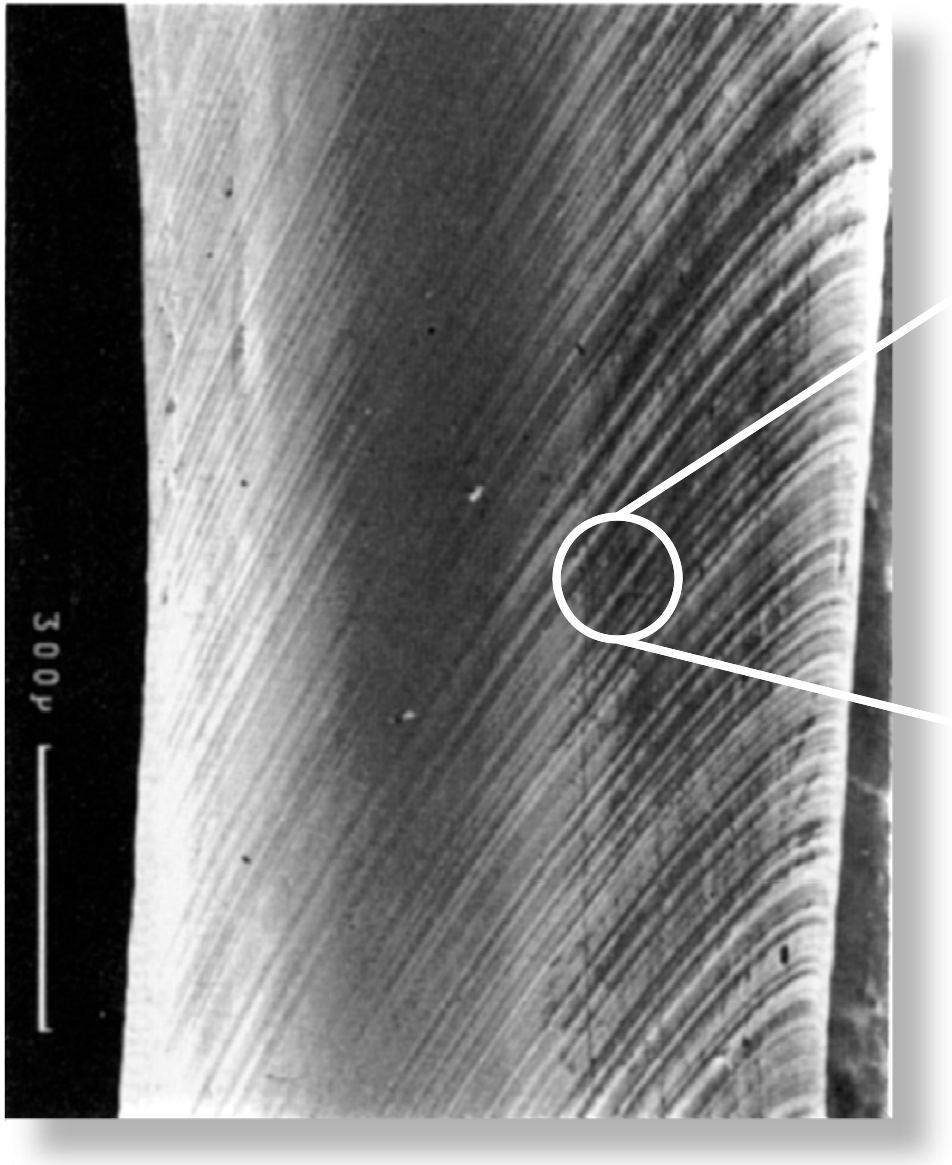

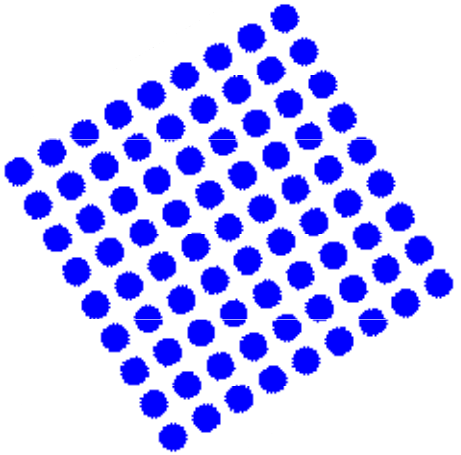

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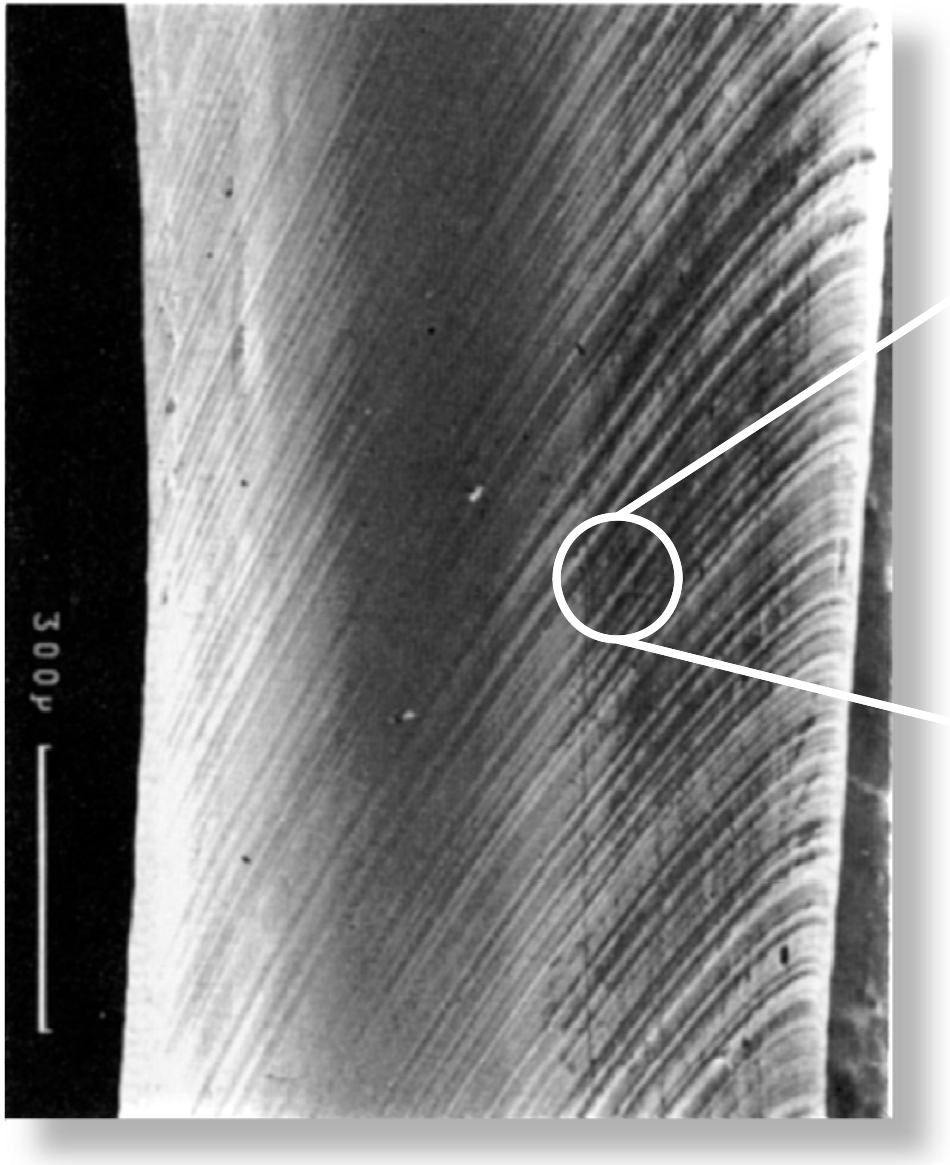
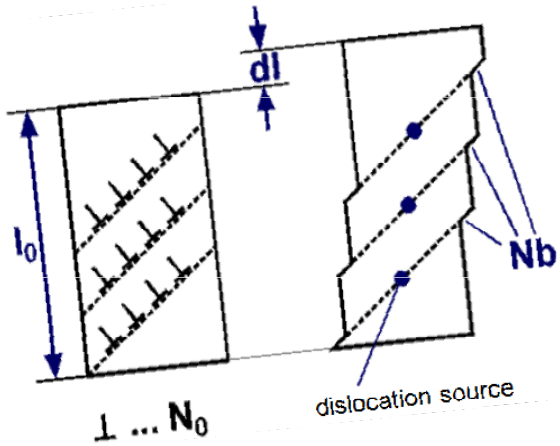
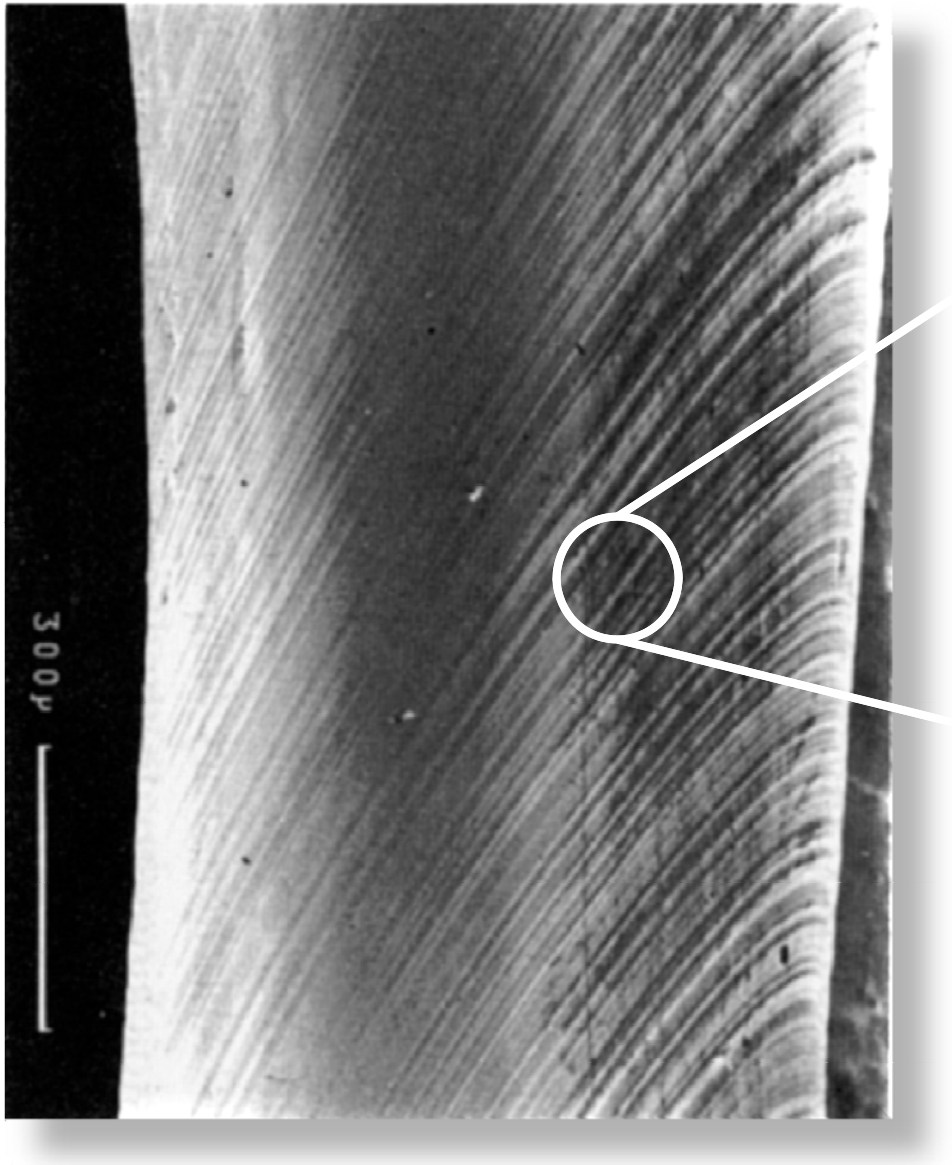
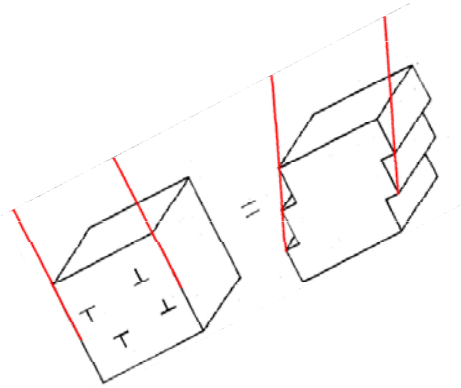




Plastic deformation of a single crystal by dislocation slip

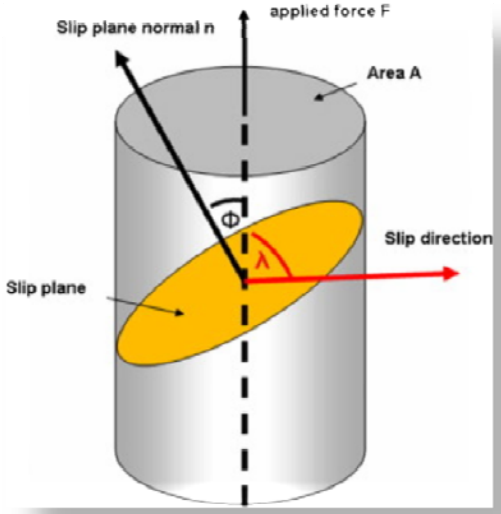




$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

Plastic deformation of a single crystal by dislocation slip

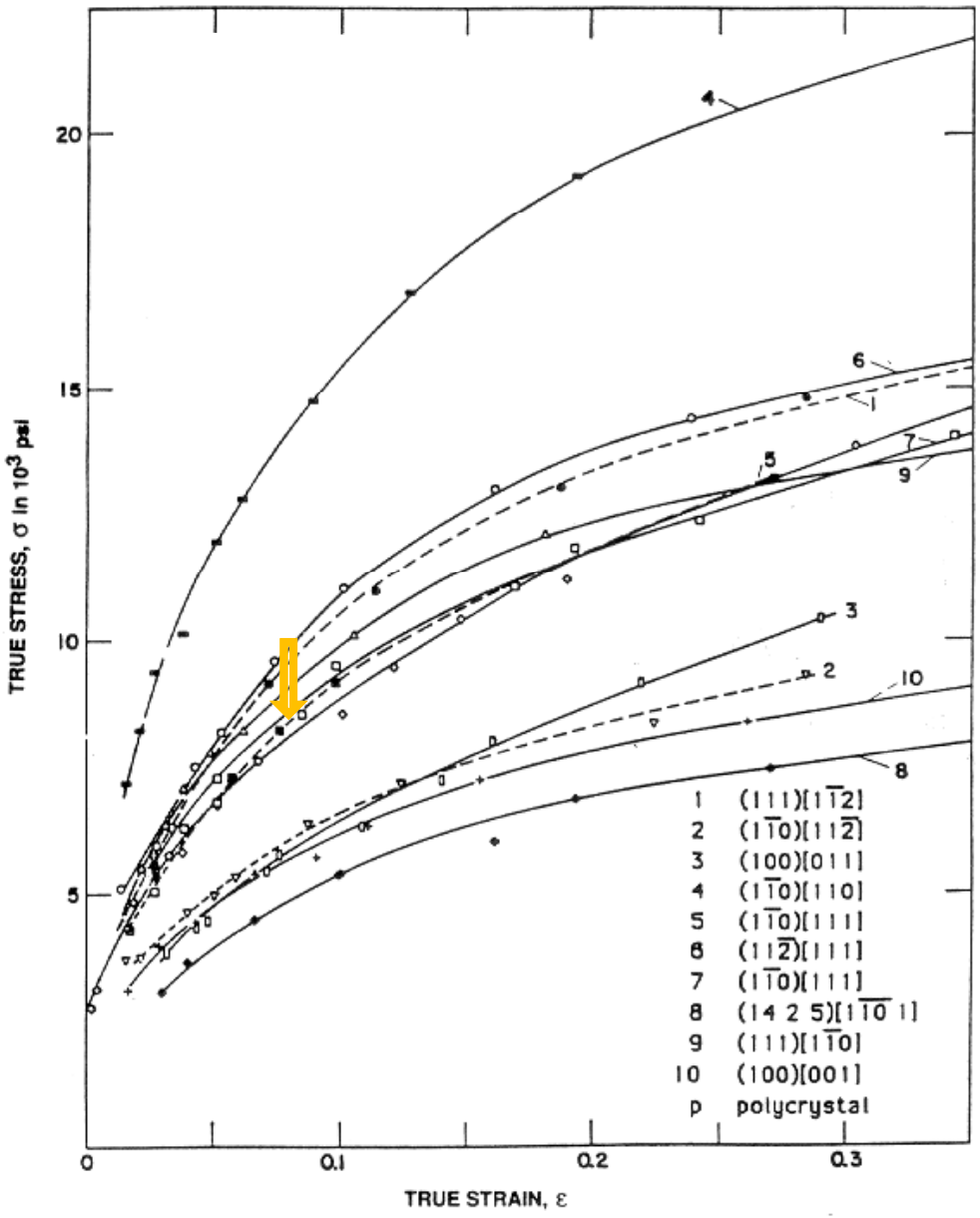
$$\tau_R = \frac{\text{resolved force acting on slip plane}}{\text{area of slip plane}} = \frac{F\cos\lambda}{A/\cos\phi} = \frac{F}{A}\cos\phi\cos\lambda$$



Schmid factor

(orientation factor for that slip system)

Plastic deformation of a single crystal by dislocation slip



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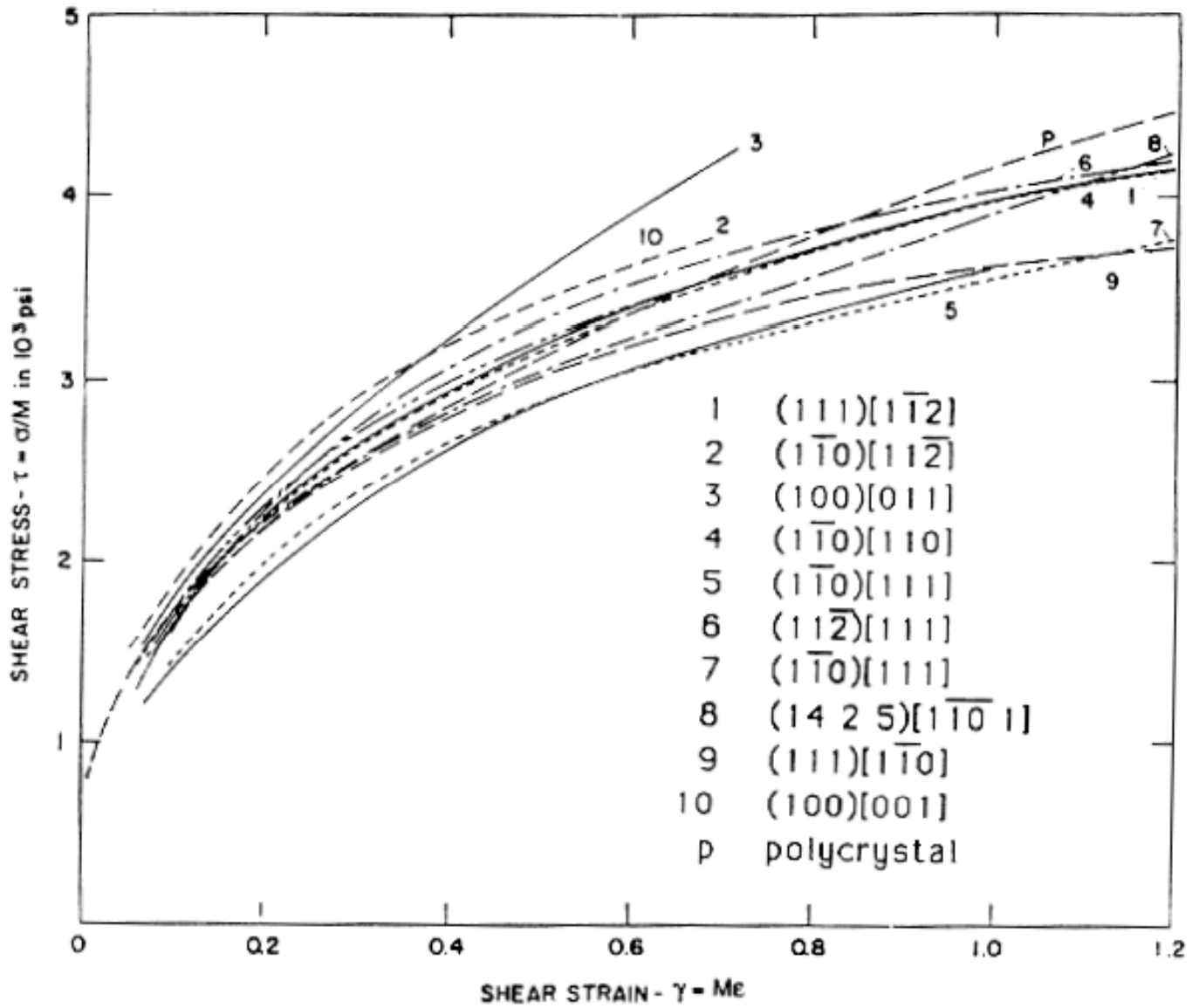
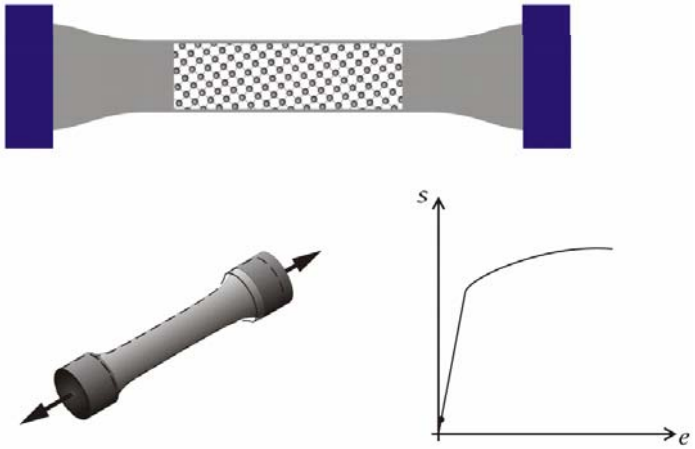
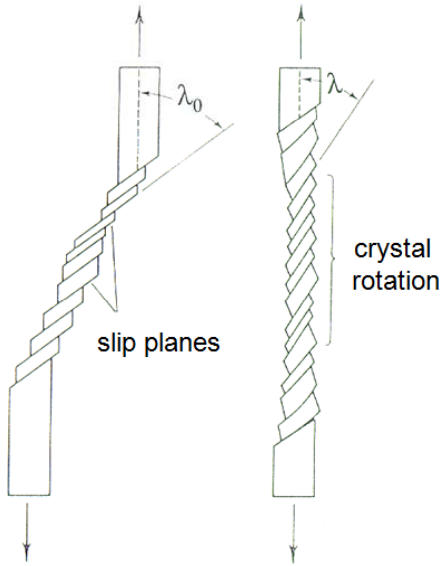
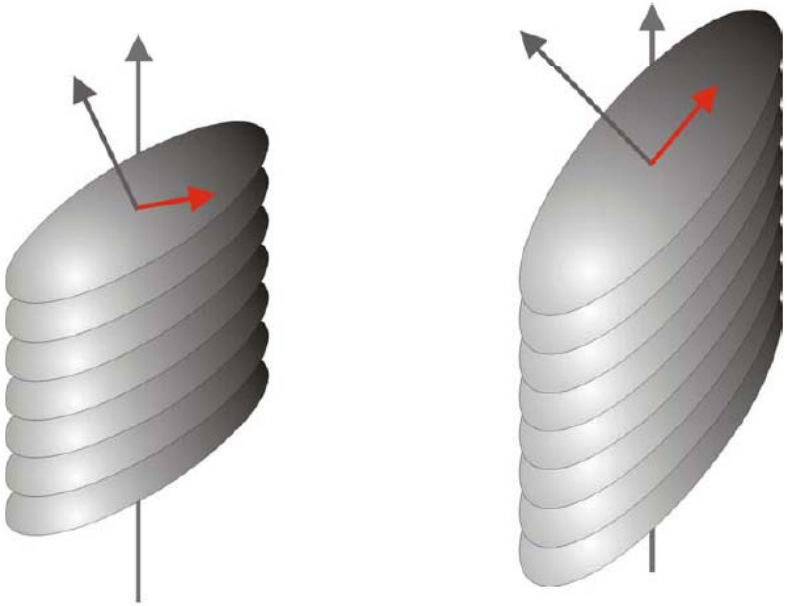


Boundary condition: determines lab frame constraints

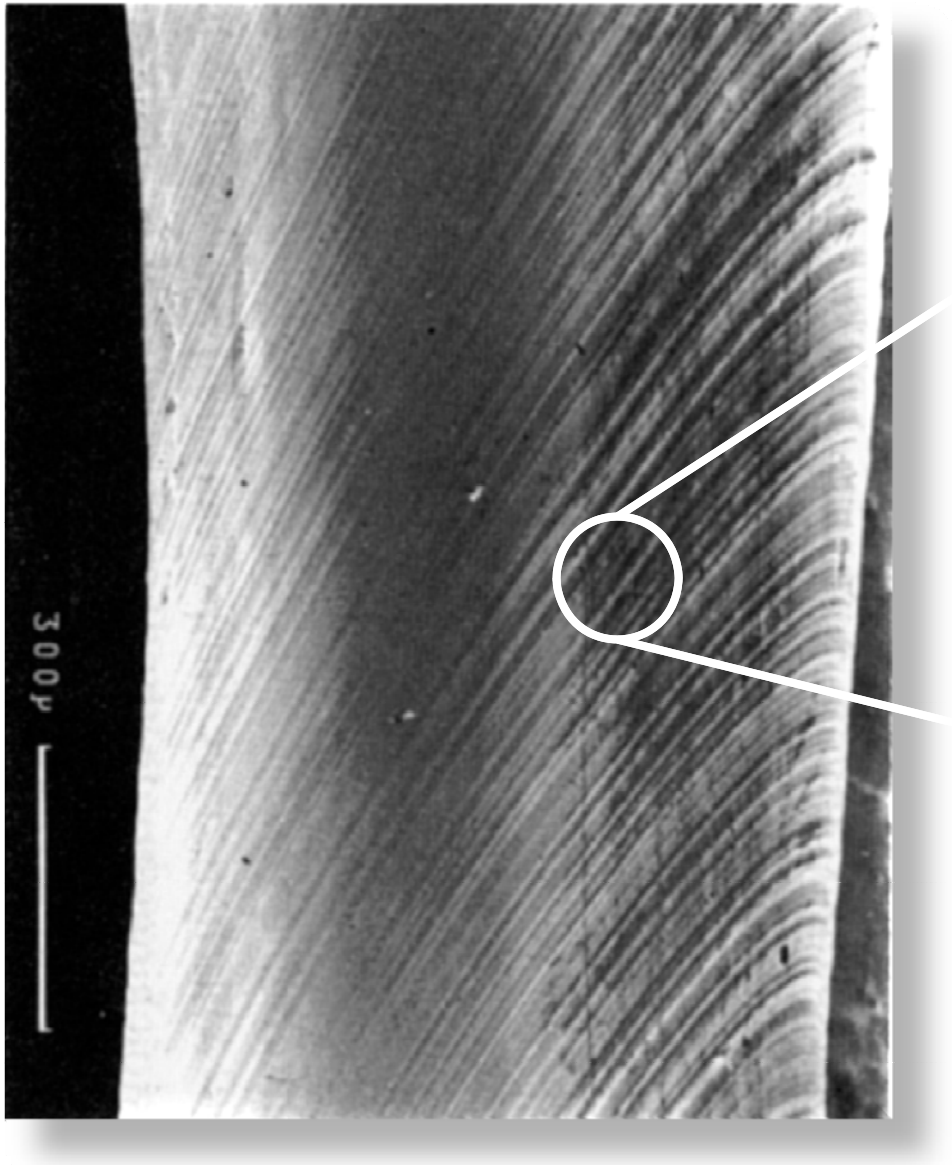


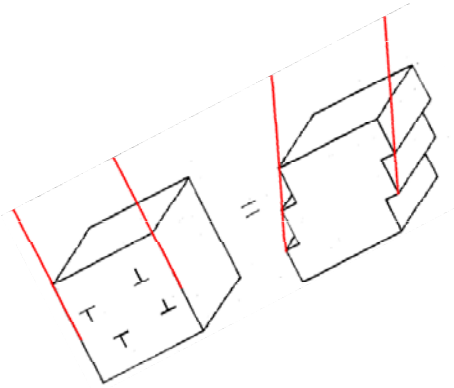


Single crystal plasticity: crystal shear and crystal rotation



Plastic deformation of a single crystal by dislocation slip





$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

Kinematics, displacement

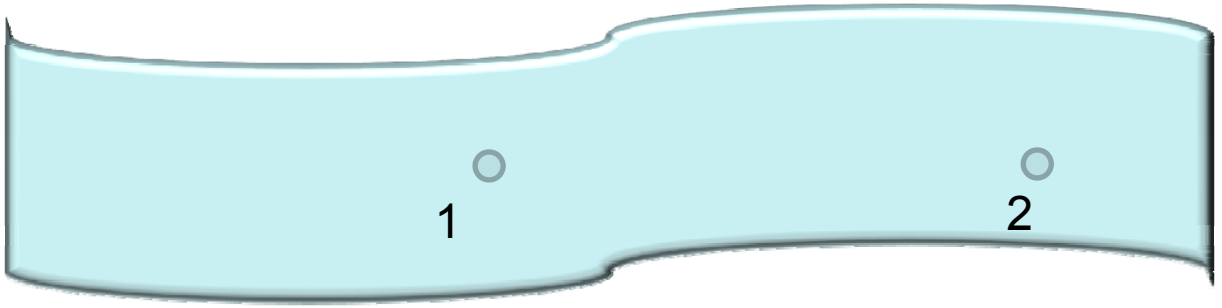
$\underline{u}=u(x,y,z)$

$\underline{u}_{(1)}(x,y,z)=\underline{u}_{(2)}(x,y,z)$

Kinematics, displacement

$\underline{u}=u(x,y,z)$

$\underline{u}_{(1)}(x,y,z)\neq\underline{u}_{(2)}(x,y,z)$



Kinematics, displacement, displacement gradient: general

Displacement vector:

$$\mathbf{u} = [u_x, u_y, u_z]$$

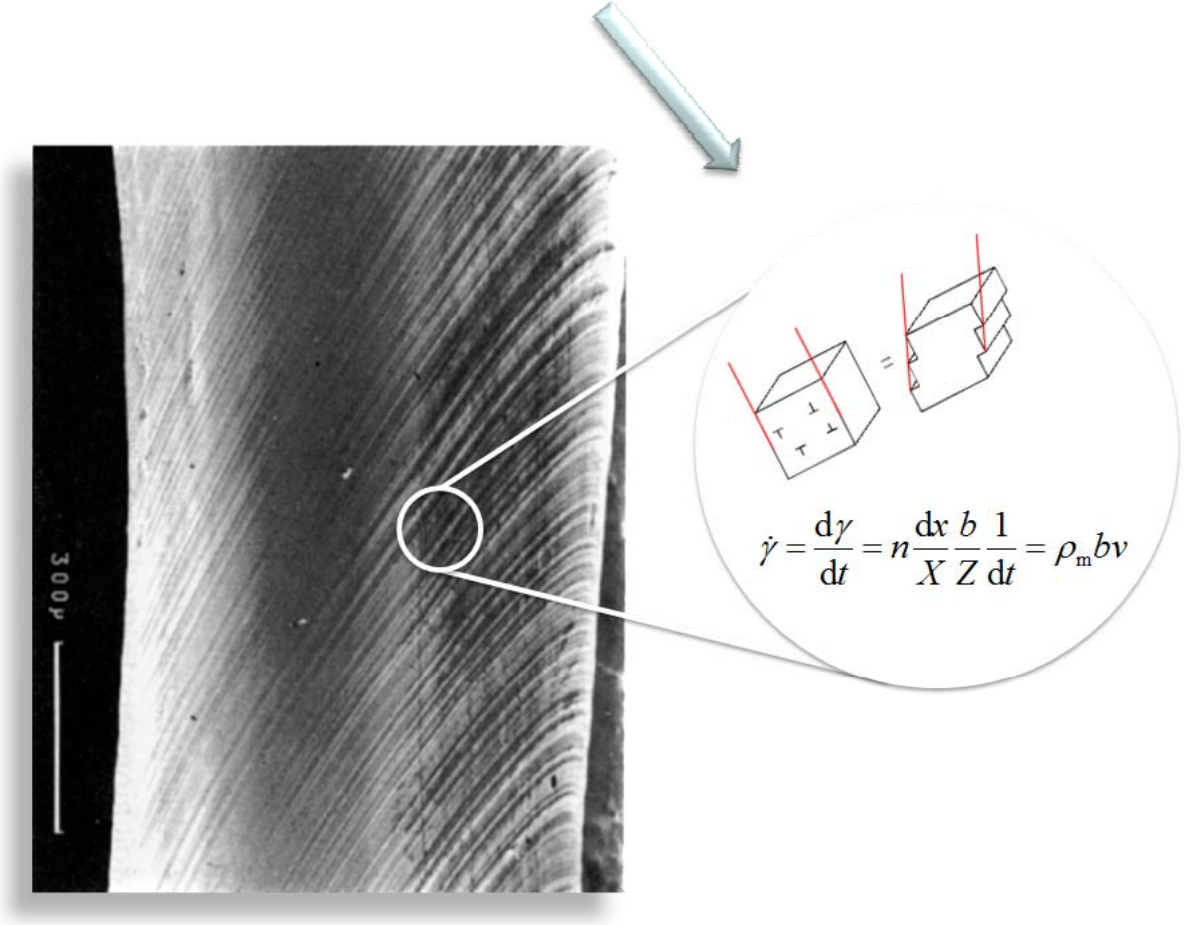
Strain tensor:

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}$$

$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)_{etc.}$$

strain rates and displacement gradients in crystals

$$\dot{\varepsilon}_{ij}^{K} = D_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} + \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{sym},s}\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{sym}} = m_{ji}^{\mathrm{sym}} = \frac{1}{2}\left(n_i b_j + n_j b_i\right)$$



Geometrical interpretation

strain rates and displacement gradients in crystals

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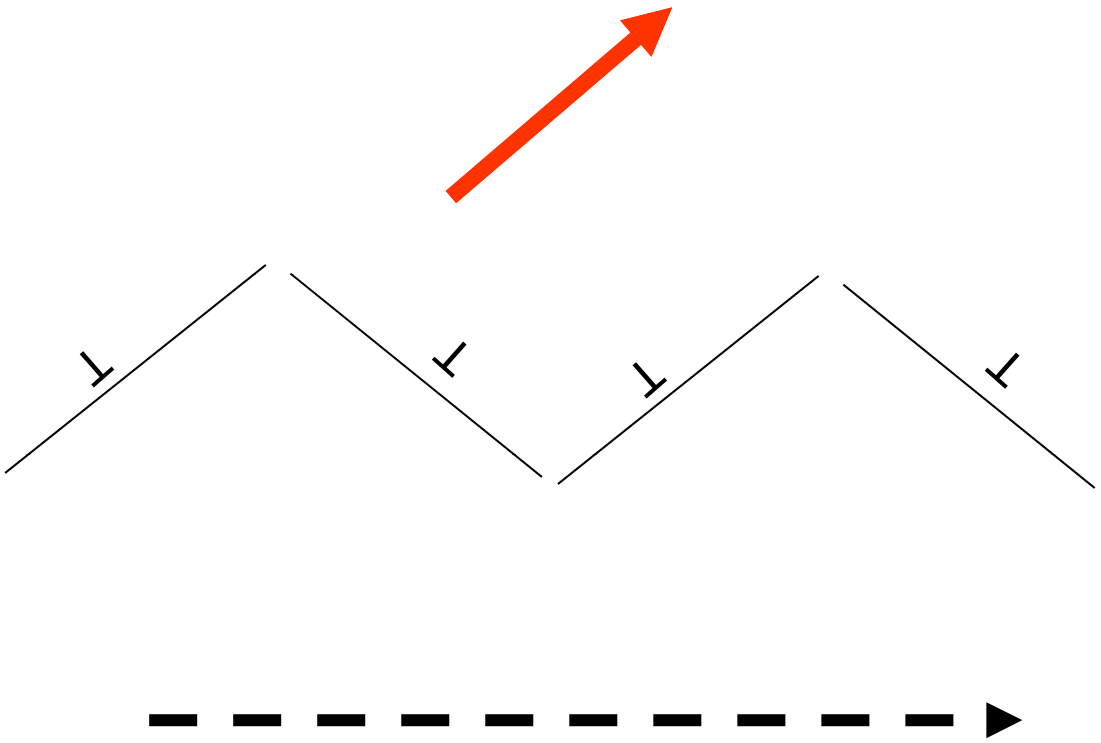

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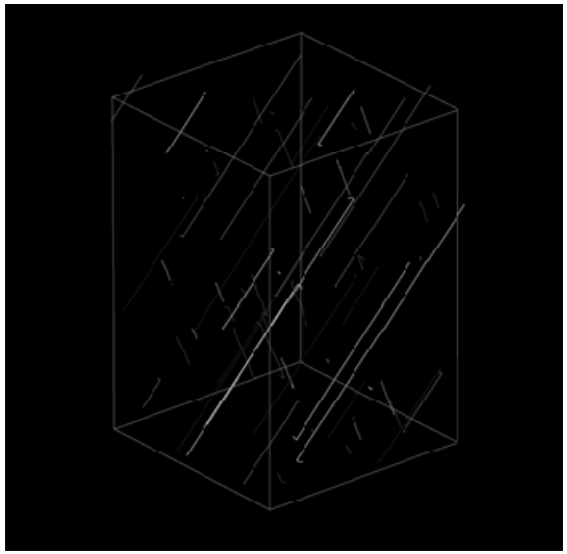
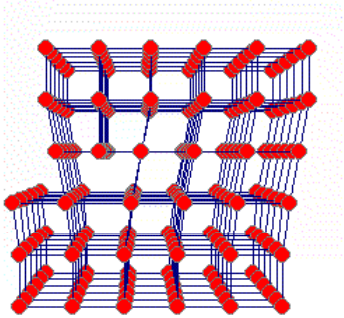
plastic spin from polar decomposition

$$\dot{\omega}_{ij}^{K} = W_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} - \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{asym},s}\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{asym}} = -m_{ji}^{\mathrm{asym}} = \frac{1}{2}\left(n_i b_j - n_j b_i\right)$$

Complex boundary conditions

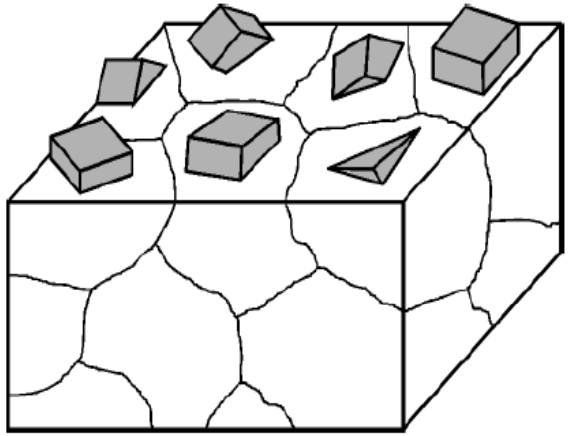


parallel loops

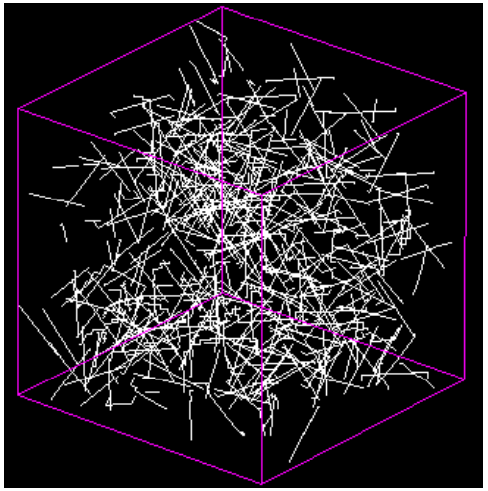


one dislocation

mesoscopic boundary conditions
(grain / orientation neighborhood)



reactions



orientation change

Simplify boundary conditions

Boundary conditions:

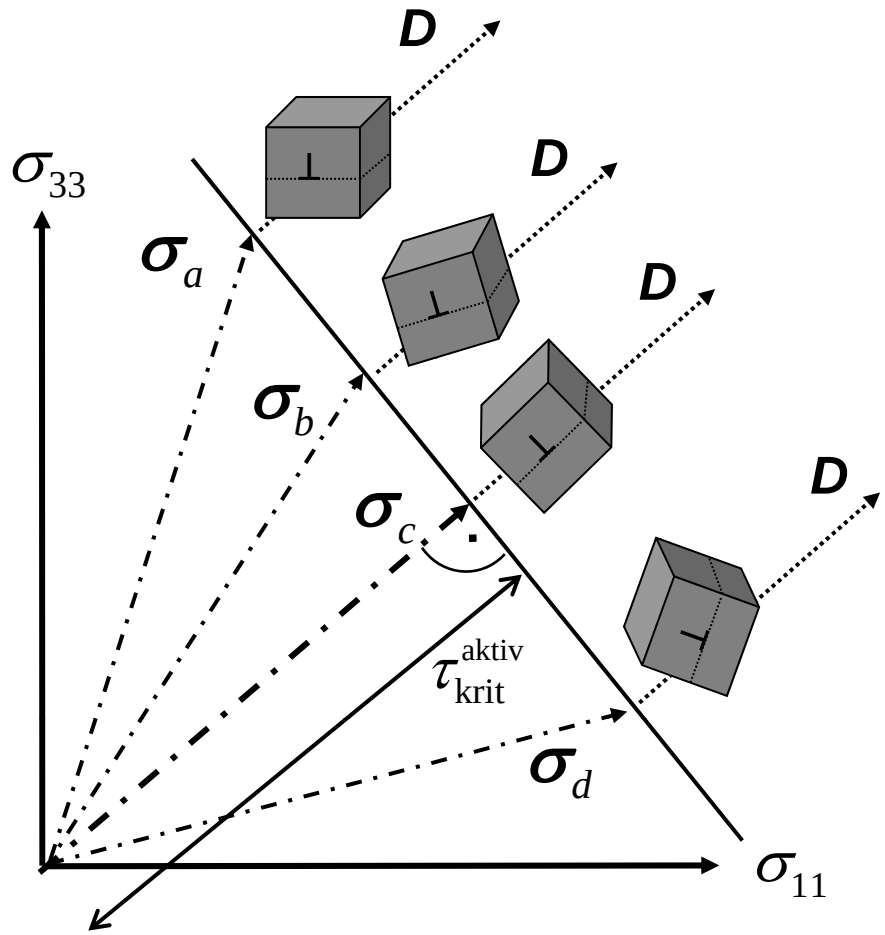
1) Upper bound treatment: iso-stress

2) Lower bound treatment: iso-strain

Iso-stress: single slip system

$$\frac{\sigma_a m_a^{sym}}{\tau_{krit}} = \frac{\sigma_b m_b^{sym}}{\tau_{krit}} = \frac{\sigma_d m_d^{sym}}{\tau_{krit}} = \frac{\sigma_c m_c^{sym}}{\tau_{krit}} = 1$$

$$|\sigma_c| < |\sigma_b| < |\sigma_d| < |\sigma_a|$$



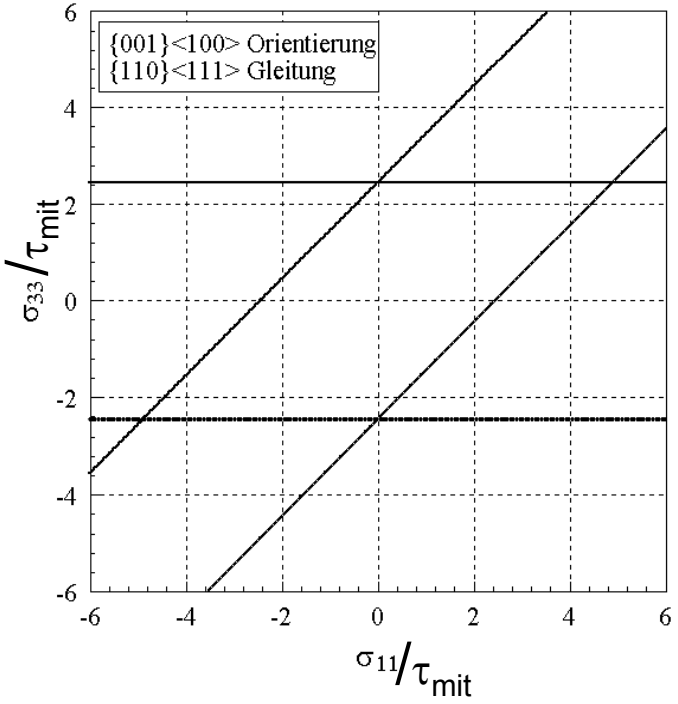
Single crystal plasticity: multiple slip (or twinning) system

slip system s

n_i^s , b_i^s

orientation factor for s

$$m_{ij}^s = n_i^s \, b_j^s$$



symmetric part

$$m_{ij}^{sym,s} = \frac{1}{2}\left(n_i^s \, b_j^s + n_j^s \, b_i^s\right)$$

rotate crystal into sample

$$m_{kl}^s = a_{ki}^c \, n_i^s \; a_{lj}^c \, b_j^s$$

symmetric part

$$m_{kl}^{sym,s} = \frac{1}{2}\left(a_{ki}^c \, n_i^s \; a_{lj}^c \, b_j^s + a_{lj}^c \, n_j^s \; a_{ki}^c \, b_i^s\right)$$

yield surface (active systems)

$$m_{kl}^{sym,s=aktiv}\sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(+)}^{s=aktiv}$$

$$m_{kl}^{sym,s=aktiv}\sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(-)}^{s=aktiv}$$

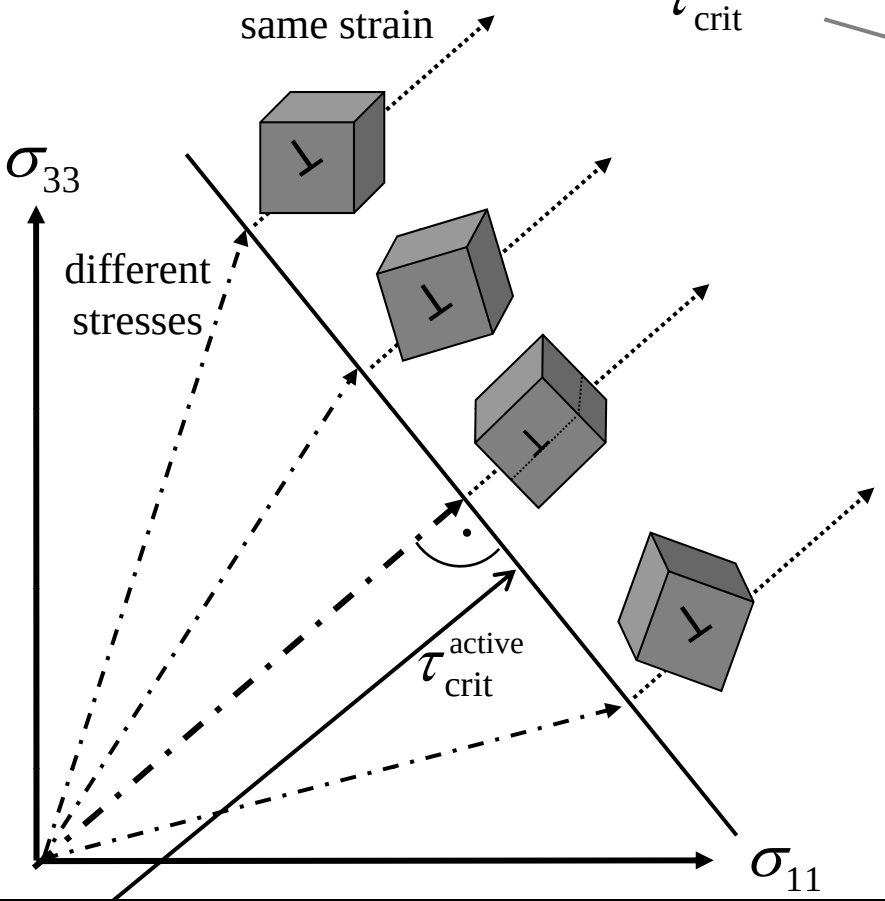
(non-active systems)

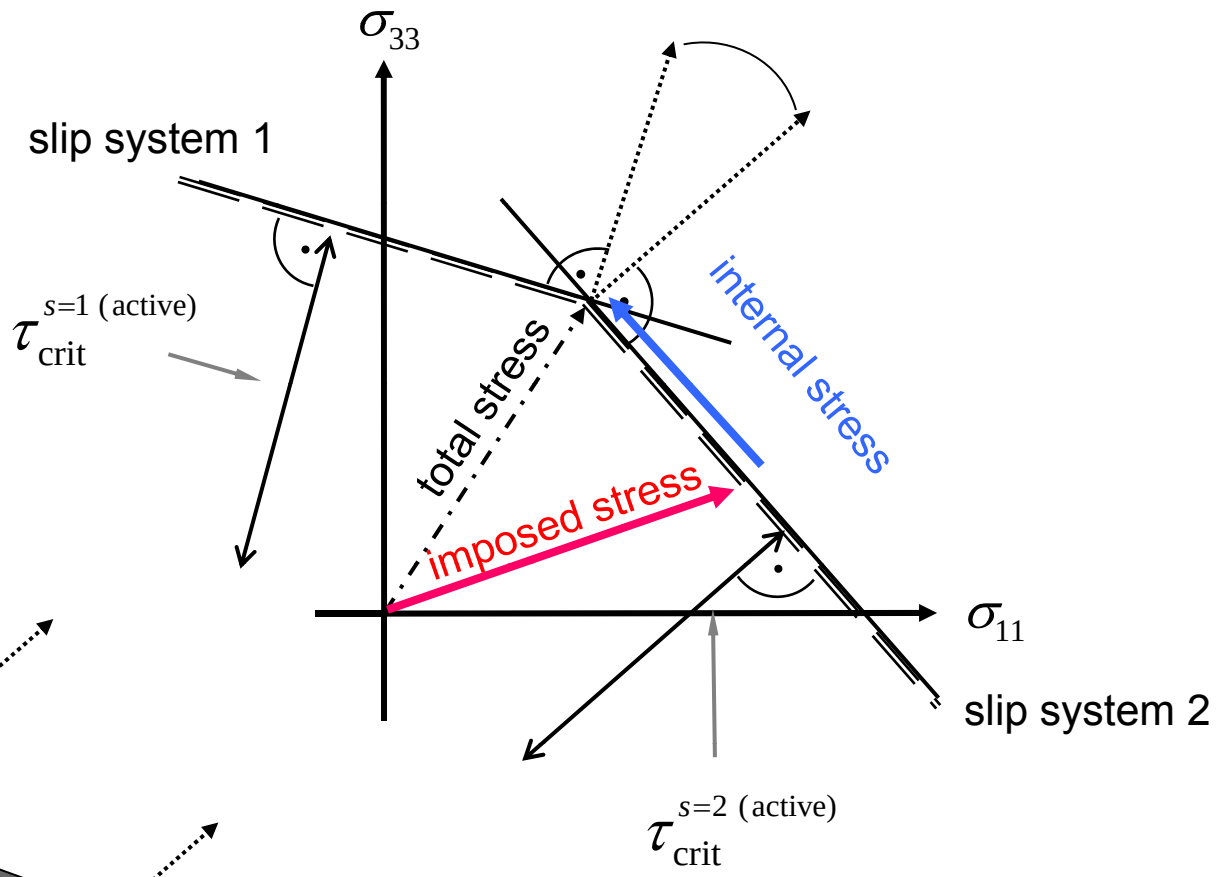
$$m_{kl}^{sym,s=inaktiv}\sigma_{kl} = \sigma_{aufg}^s < \tau_{krit,(\pm)}^{s=inaktiv}$$

Single crystal yield surface

1 crystal, 1 slip system:

$$a_{ik} n_k a_{jl} b_l \sigma_{ij} = \tau^{crit}$$

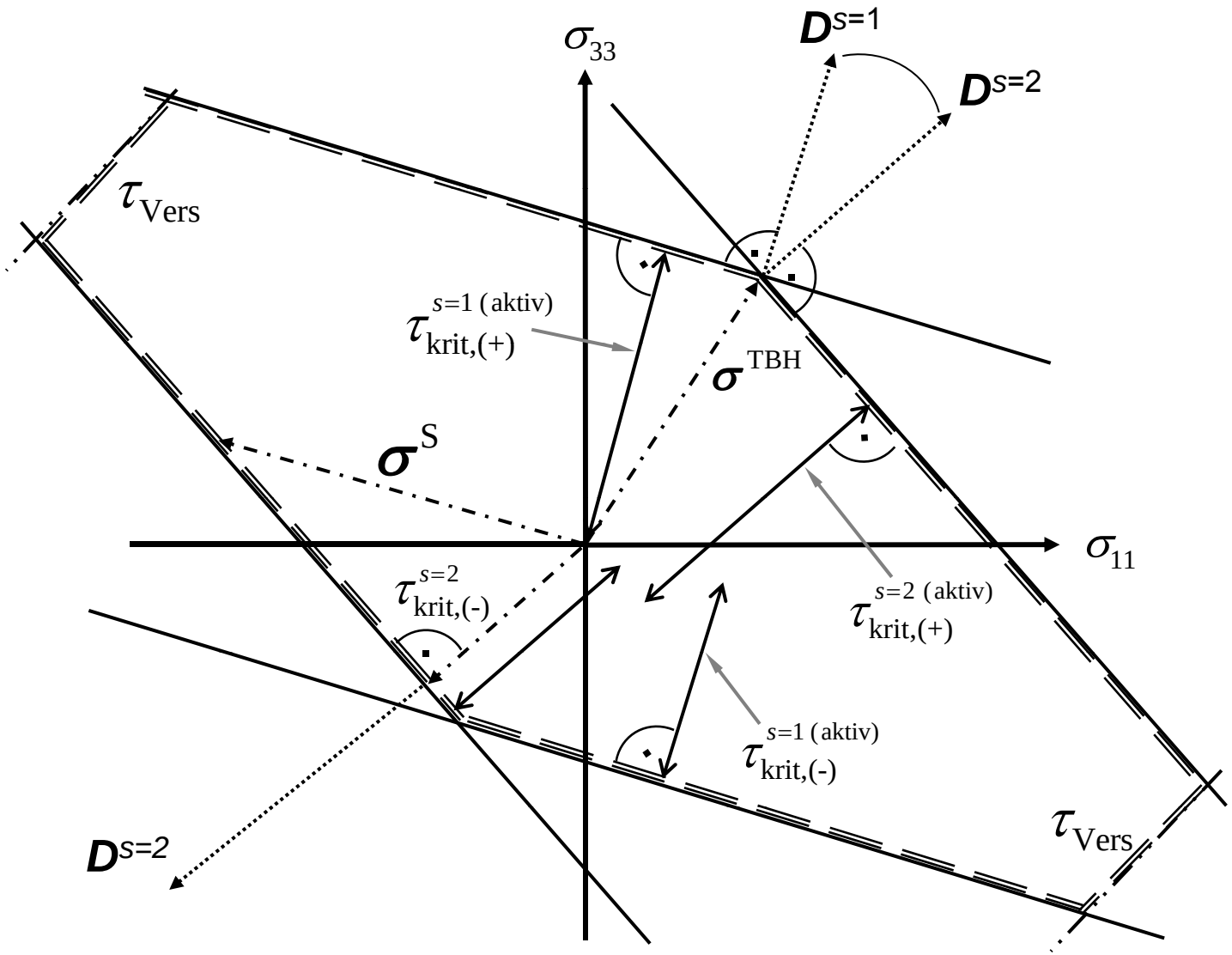




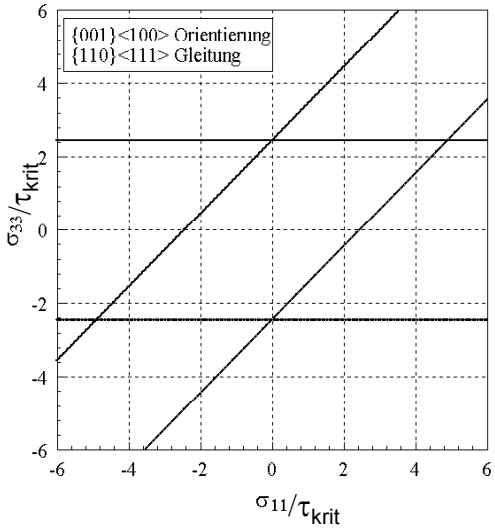
1 crystal, 2 slip systems:

$$a_{ik} n_k^s a_{jl} b_l^s \sigma_{ij} = \tau^{crit}$$

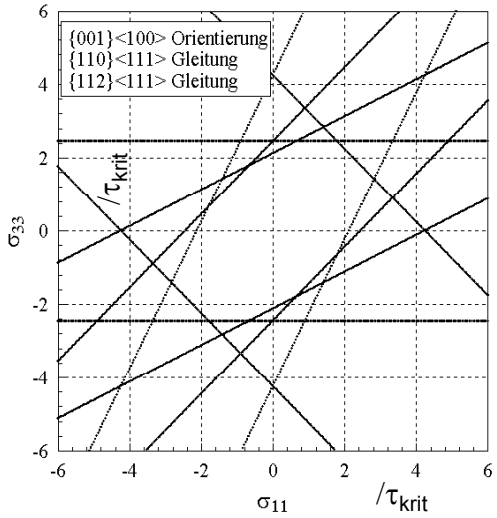
Iso-stress: multiple slip (or twinning) system



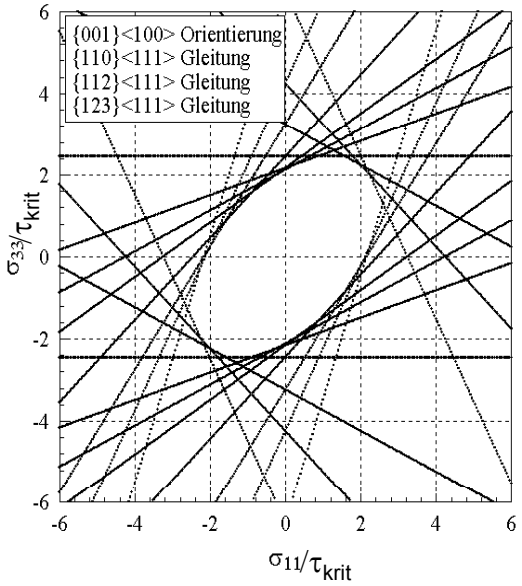
Single crystal plasticity



bcc, fcc,
Section in
stress space



Bcc: 24 systems



BCC, 48 systems

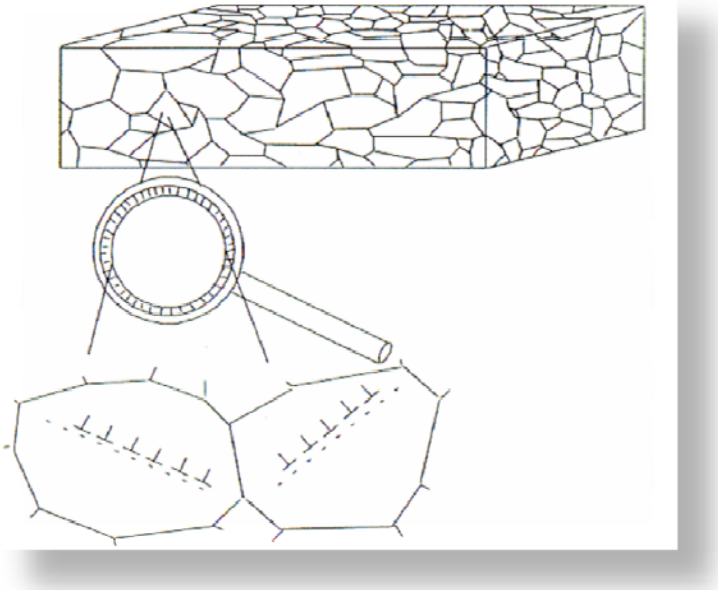
Simplify boundary conditions

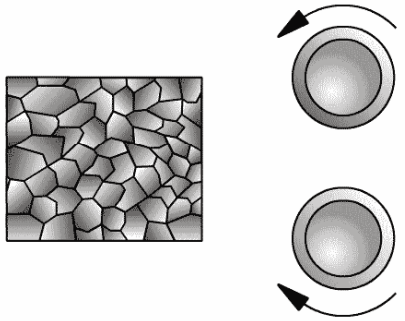
Boundary conditions:

1) Upper bound treatment: iso-stress

2) Lower bound treatment: iso-strain

The Taylor Model



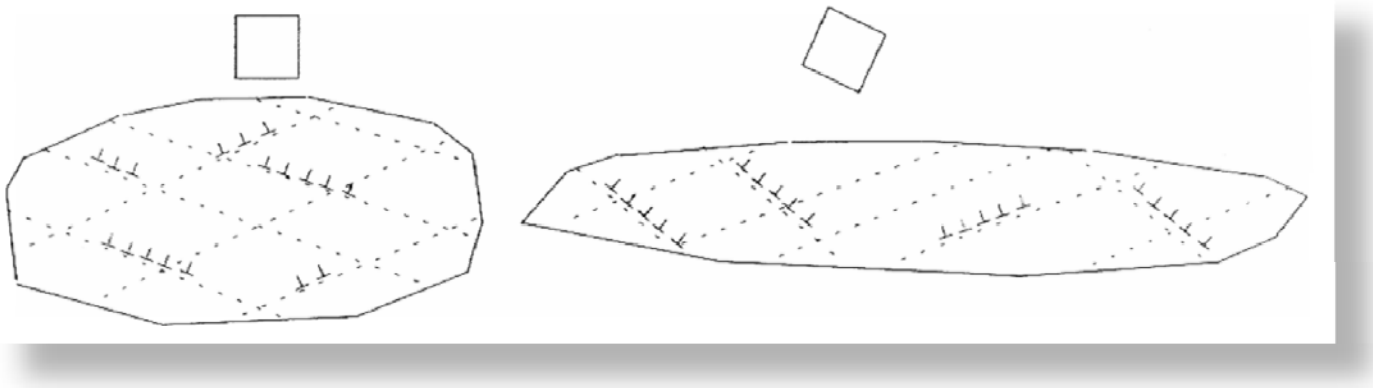


Cold Rolling

$$\varepsilon_{ij} = \frac{1}{2}\sum_{s=1}^{5}\left(n_i^s b_j^s + n_j^s b_i^s\right)\gamma^s$$

Crystal yield surface, Taylor Bishop-Hill

$$\varepsilon_{ij} = \frac{1}{2}\sum_{s=1}^{5}\left(n_i^s b_j^s + n_j^s b_i^s\right)\gamma^s$$

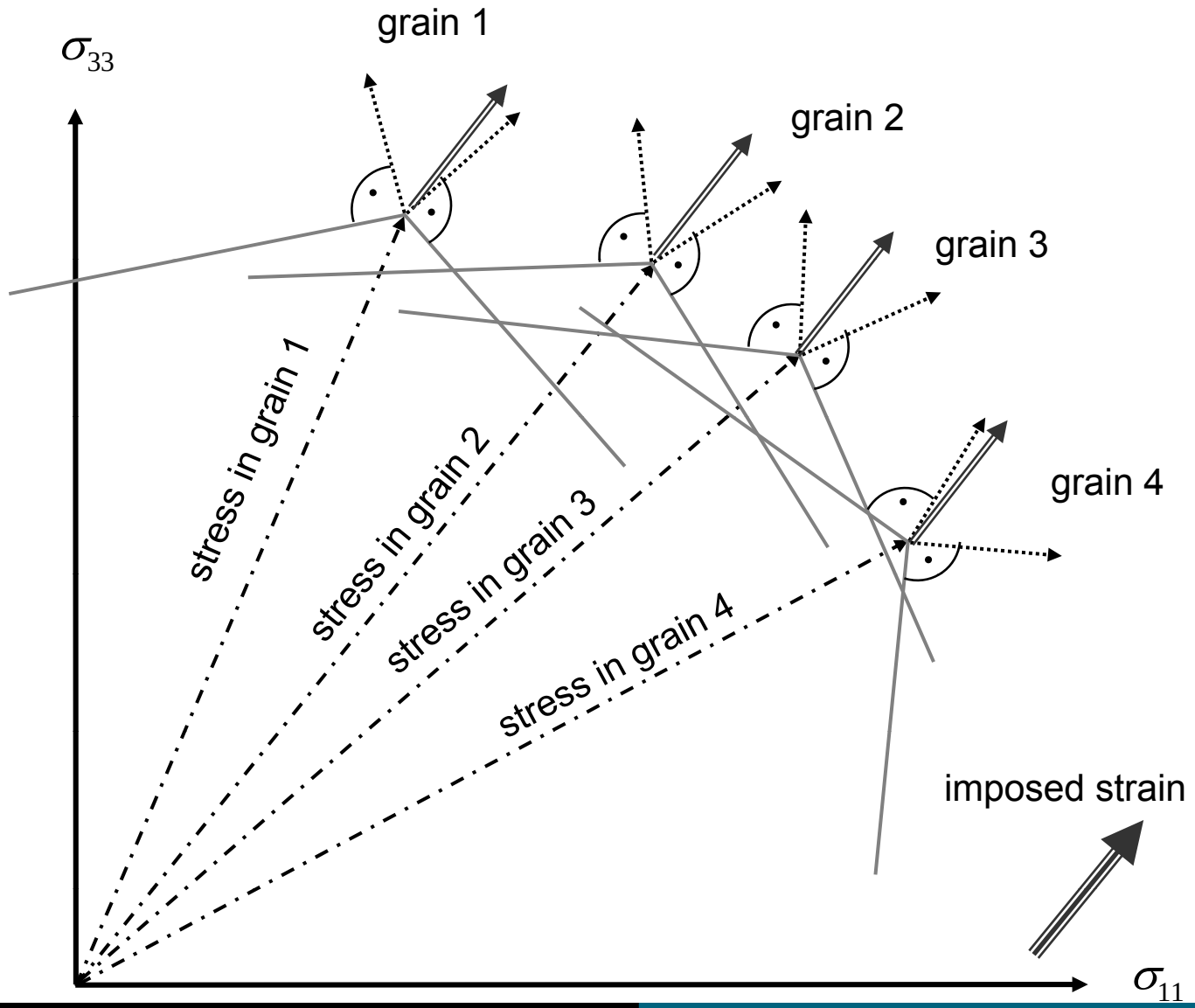


plastic spin from polar decomposition

$$\dot{\omega}_{ij}^K = W_{ij}^K = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} - \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{asym},s}\dot{\gamma}^s$$

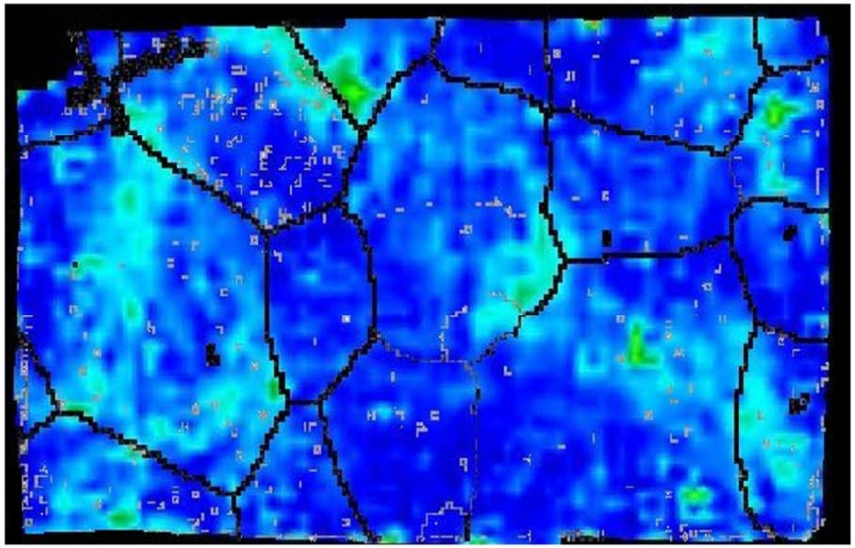
Crystal yield surface, Taylor Bishop-Hill

Many crystals, many slip systems:

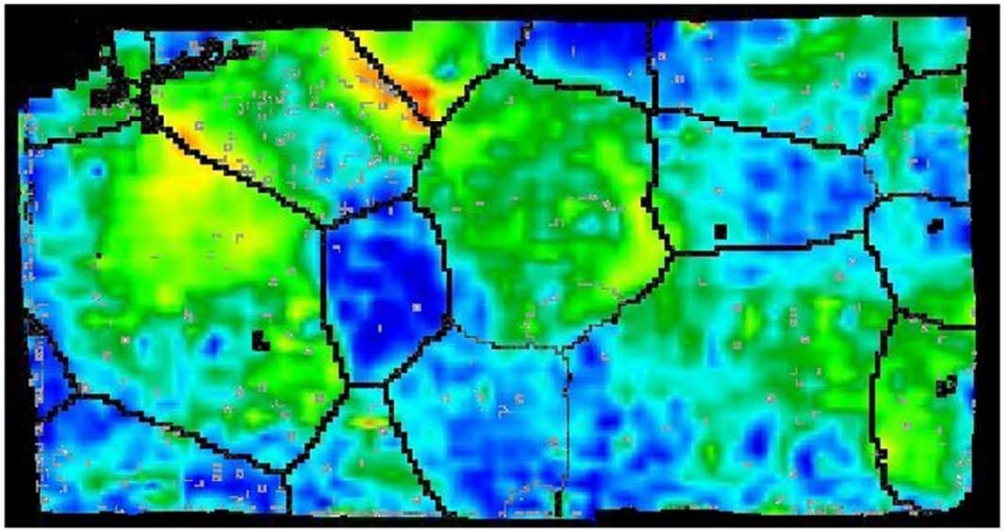


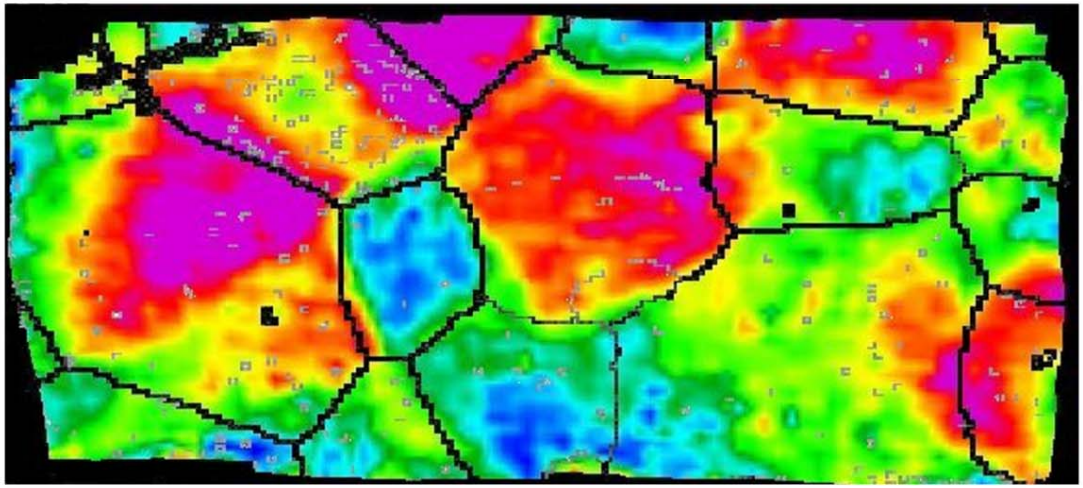
Homogeneity and boundary conditions – meso-scale

3%



8%





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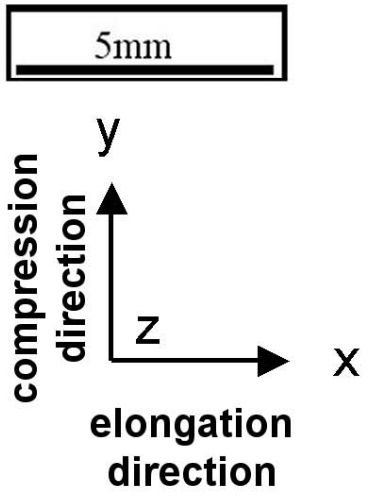


accumulated von Mises strain

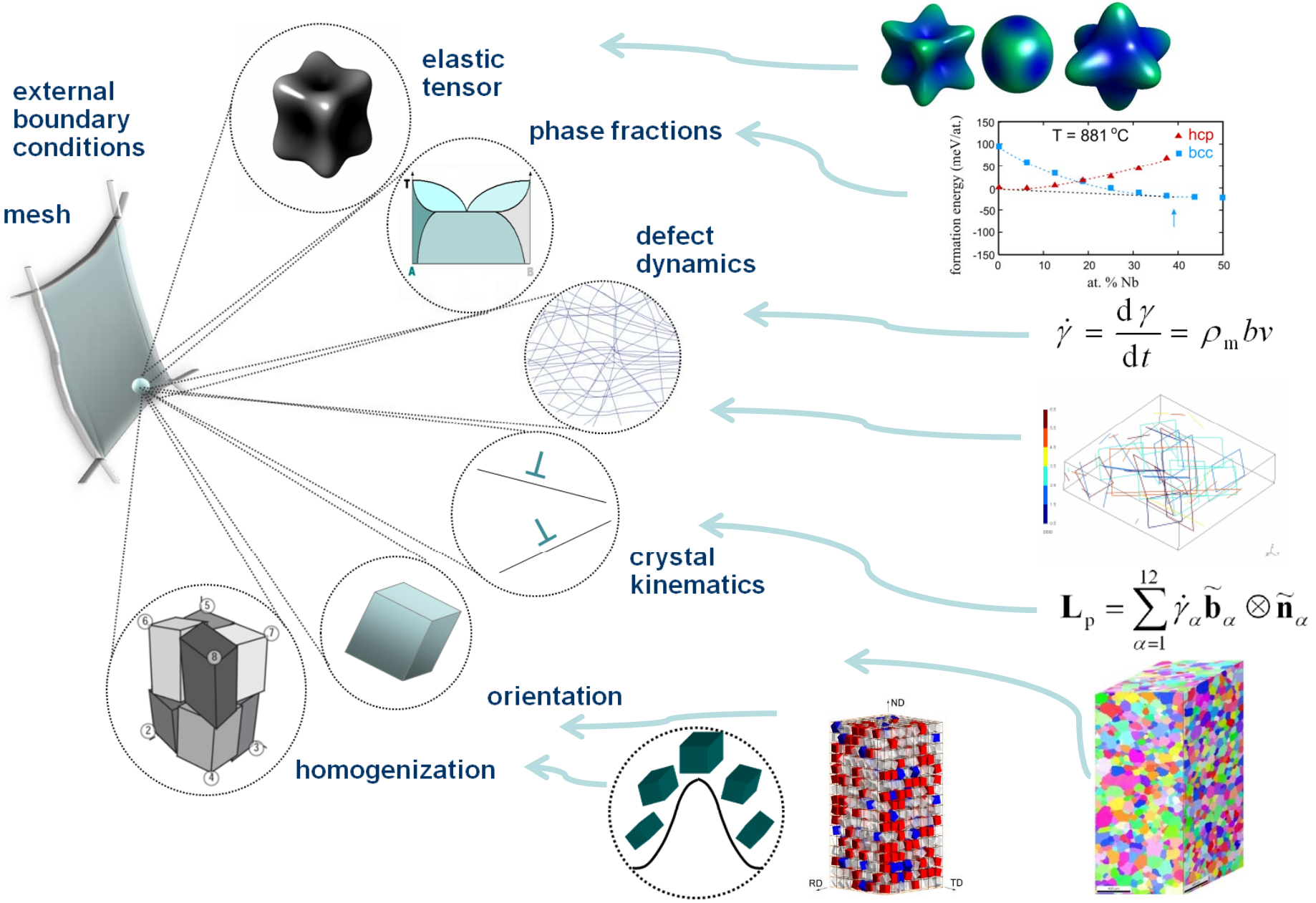
Simplify boundary conditions

Boundary conditions:

1) Upper bound treatment: iso-stress (strain not compatible)

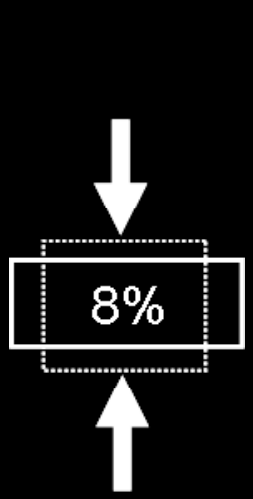
2) Lower bound treatment: iso-strain (forces not in equilibrium)

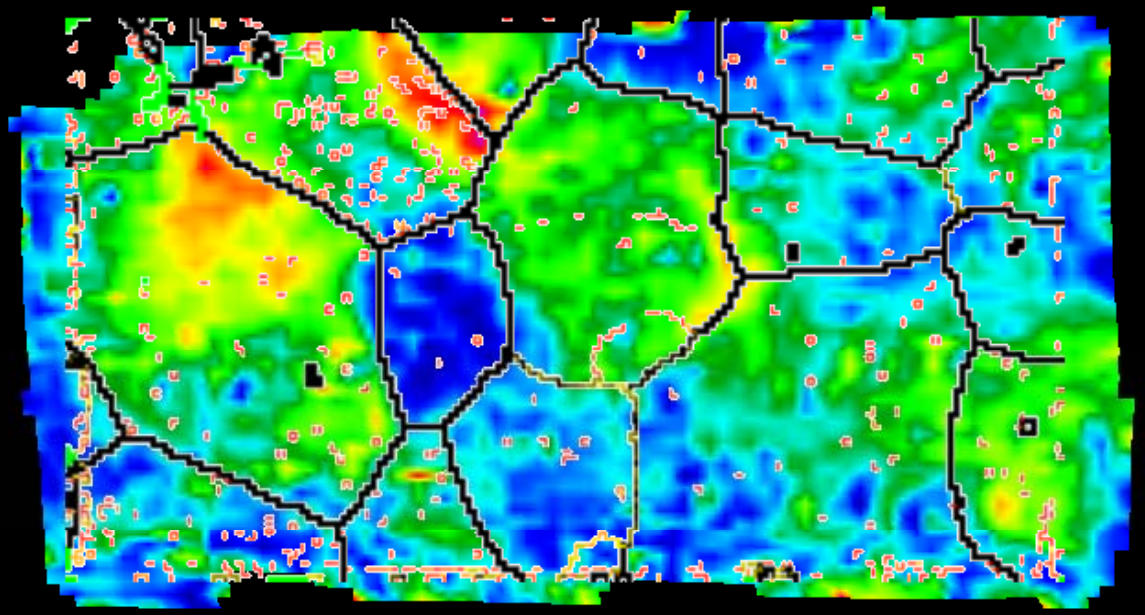
Multiscale crystal plasticity FEM or FFT

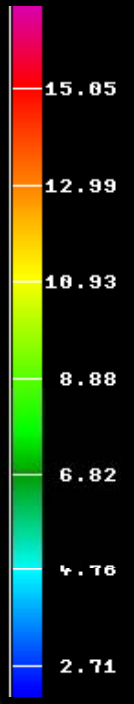


Raabe, Zhao, Park, Roters: Acta Mater. 50 (2002) 421

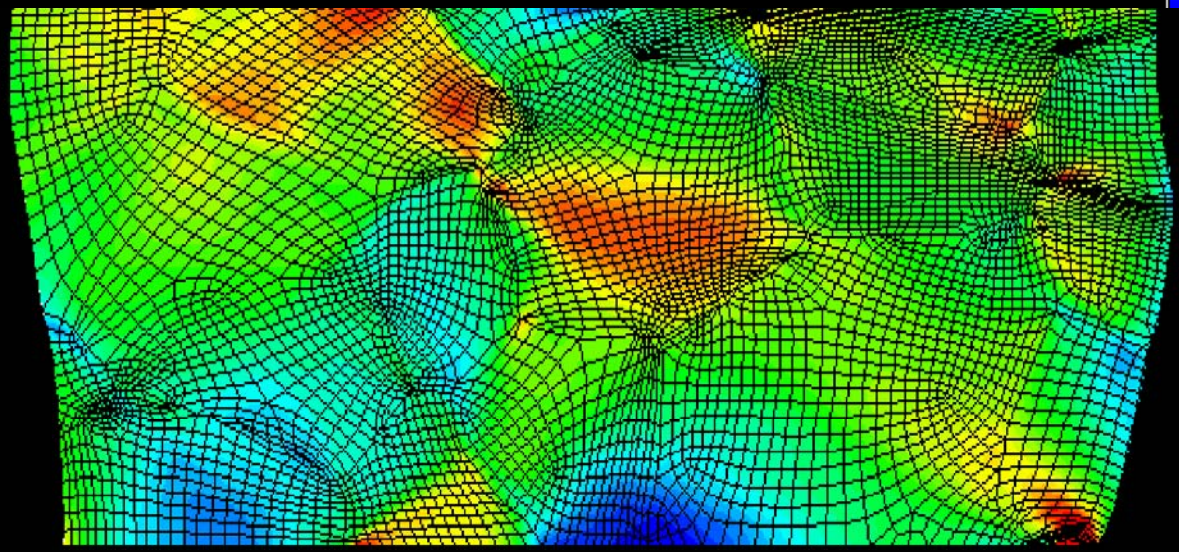
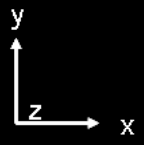
Crystal Mechanics FEM, grain scale mechanics (2D)







Experiment
(DIC, EBSD)
v Mises strain



Simulation
(CP-FEM)
v Mises strain