The crystalline structure of metals: why does it matter for crystal mechanics ?

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Class 2016

Contact, website and class days

class times

Friday, 10:15 am – 2 pm at IMM / RWTH

Course Lecturers:
Dr. S. Sandlöbes, Prof. R. Svendsen,
Dr. P. Shanthraj, Dr. S.-L. Wong, Prof. D. Raabe

Notes at:

http://www.dierk-raabe.com/teaching/

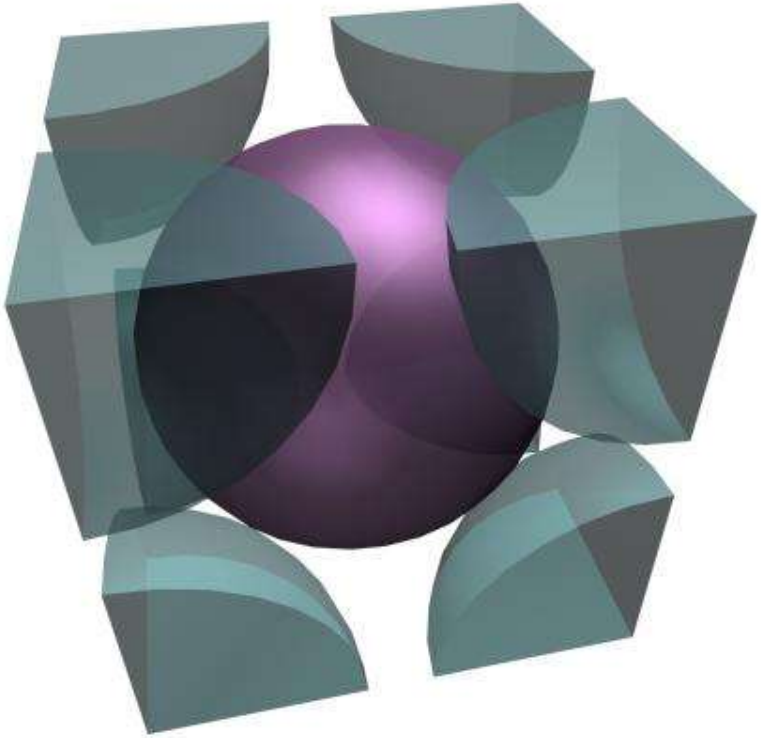
Contact, website and class days

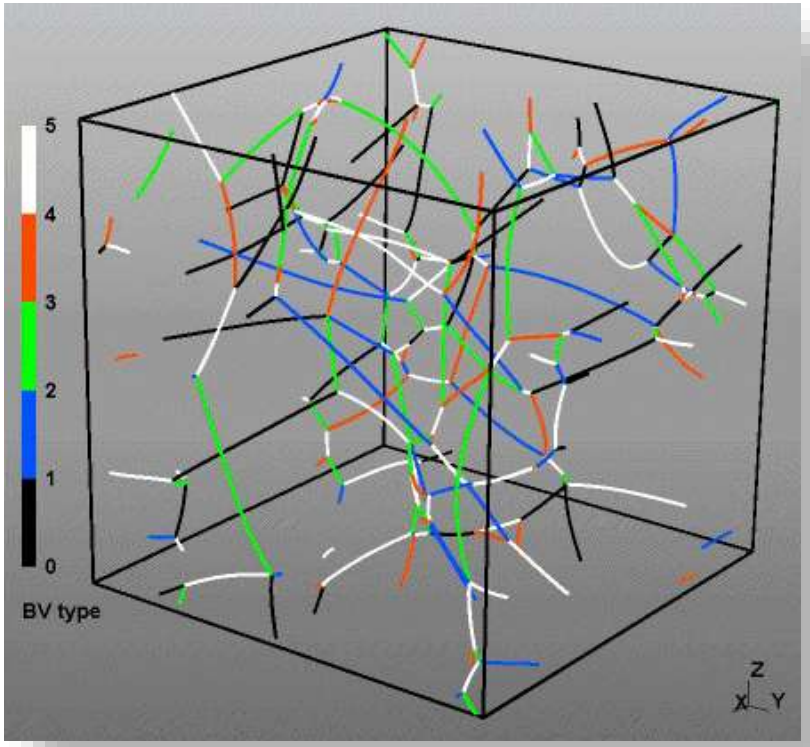
Date / Location	Topics	Lecturer
21. April 2017 **IMM / RWTH**	Introduction to materials micromechanics, multiscale problems in micromechanics, case studies, crystal structures and defects, relation to products and manufacturing	Raabe
28. April 2017 **IMM / RWTH**	Discrete and statistical dislocation dynamics, Crystal micromechanics, single crystal mechanics, yield surface mechanics, polycrystal models, Taylor model	Raabe
5. May 2017 **IMM / RWTH**	Athermal phase transformations in micromechanics	Wong
12. May 2017 **IMM / RWTH**	Fracture mechanics, Introduction to FEM	Shanthraj
19. May 2017 **MPI / Düsseldorf**	Micromechanics of polymers and biological (natural) composites	Raabe
26. May 2017 **IMM / RWTH**	Fatigue of materials	Sandlöbes
2. June 2017 **IMM / RWTH**	Mathematical micromechanics: Review of elasticity theory	Svendsen
9. June 2017 **IMM / RWTH**	Volterra dislocation theory	Svendsen
16. June 2017 **IMM / RWTH**	Dislocations and micromechanics in hexagonal materials	Sandlöbes
23. June 2017 **IMM / RWTH**	Dislocation interaction modeling	Svendsen
30. June 2017 **IMM / RWTH**	Partial and extended dislocations	Svendsen
7. July 2017 **IMM / RWTH**	Peierls-Nabarro disocation theory and dislocation core modeling	Svendsen

Crystal dislocations: Relationship between lattice and defects

What is the connection between ‚simple ‘ structure data and complex dislocation structures?

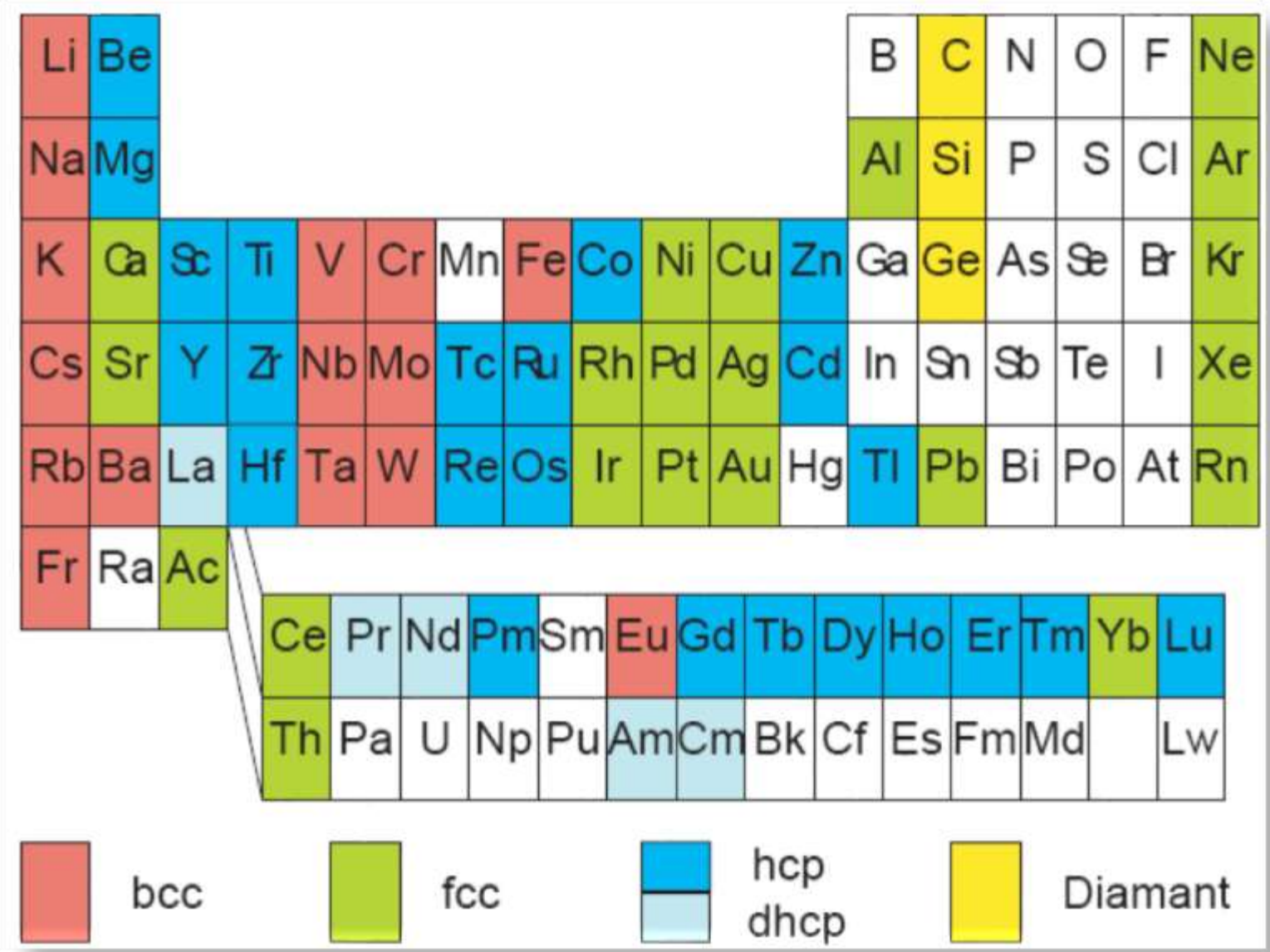
Why is the crystal lattice relevant for understanding complex dislocation structures?





Body centered cubic (bcc) lattice structure

How frequently do certain crystal structures occur in the PSE?



Lattice parameters

FCC: Face centered cubic close packed, (a)	Hexagonal close packed (a, c)	BCC: Body centered cubic (a)
Cu (3.6147)	Be (2.2856, 3.5832)	Fe (2.8664)
Ag (4.0857)	Mg (3.2094, 5.2105)	Cr (2.8846)
Au (4.0783)	Zn (2.6649, 4.9468)	Mo (3.1469)
Al (4.0495)	Cd (2.9788, 5.6167)	W (3.1650)
Ni (3.5240)	Ti (2.506, 4.6788)	Ta (3.3026)
Pd (3.8907)	Zr (3.312, 5.1477)	Ba (5.019)
Pt (3.9239)	Ru (2.7058, 4.2816)	
Pb (4.9502)	Os (2.7353, 4.3191)	
	Re (2.760, 4.458)	

Crystal dislocations: Relationship between lattice and defects

Why is the crystal lattice relevant for understanding complex dislocation structures?

Densely packed planes: glide planes; densely packed translation shear vectors: Burgers vectors

Twinning systems

Stacking fault energy: planar dislocation cores, cross slip, recovery, annihilation, Suzuki effect, twinning, strain hardening, stair rod dislocations, reactions

Shockley partial dislocations (*b* = a/6<112>)

Crystal dislocations: Relationship between lattice and defects

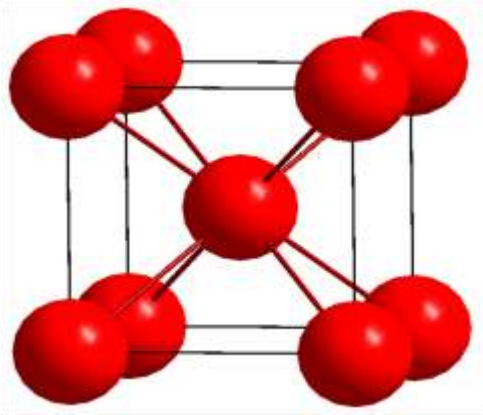
Special properties of the 3 main lattice types regarding plasticity defects

FCC: stacking fault energy can vary from very low values (α-Brass- 30 wt% Zn in Cu; TWIP steels: ≈ 20 mJ/m^2) to very high values (Al : ≈ 180 mJ/m^2): Regarding lattice defects in plasticity FCC and HCP is not a 'homogeneous' or unique crystal structure

Hex: hcp or hex?; c/a ratio determines slip systems and twinning: some hex metals are very brittle (Mg) and some are rather ductile (Ti)

BCC: non-close packed planes: pencile glide behavior; multiple slip systems: {110}; {112}; {123}; complex core of dislocation; twinning vs. anti-twinning glide sense

Crystal structure: BCC



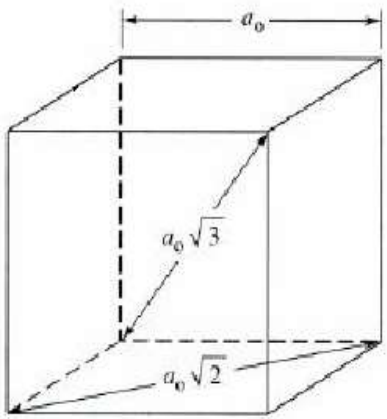
atoms per cell = $(8 \times 1/8) + 1 = 2$

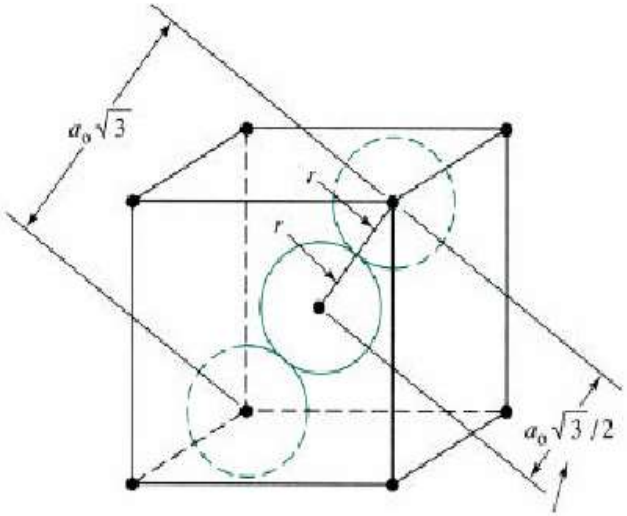
coordination number = $4 + 4 = 8$

atomic packaging = 0.68

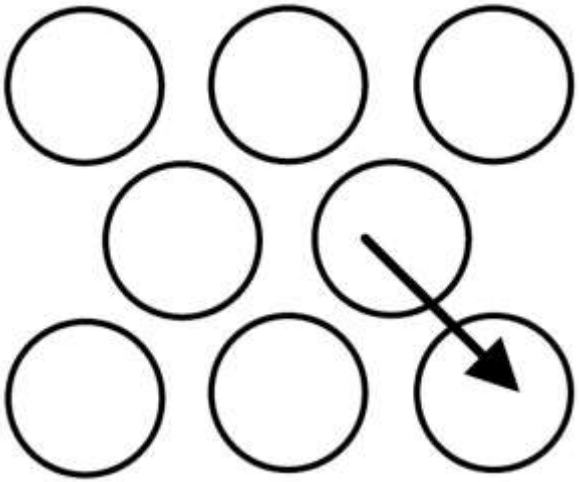
$$4r = \sqrt{3}a$$

$$\boxed{a = \frac{4}{\sqrt{3}} r}$$





Glide plane: BCC

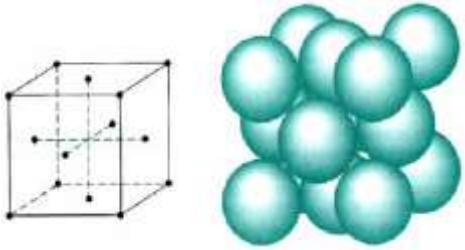


Crystal structure: FCC

atoms per cell = (8 x 1/8) + (6 x ½) = 4

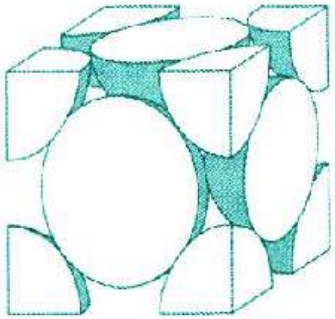
coordination number = 4 + 4 + 4 = 12

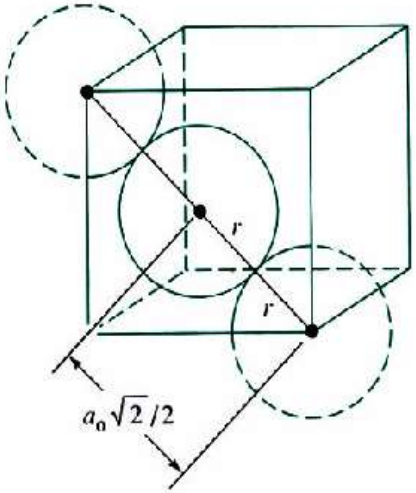
atomic packaging = 0.74



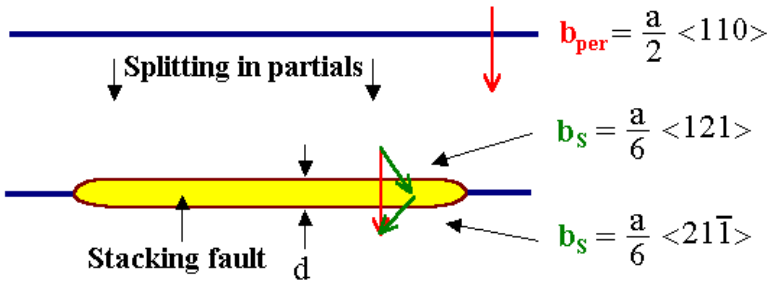
$$4r = \sqrt{2}a$$

$$a = 2\sqrt{2}r$$



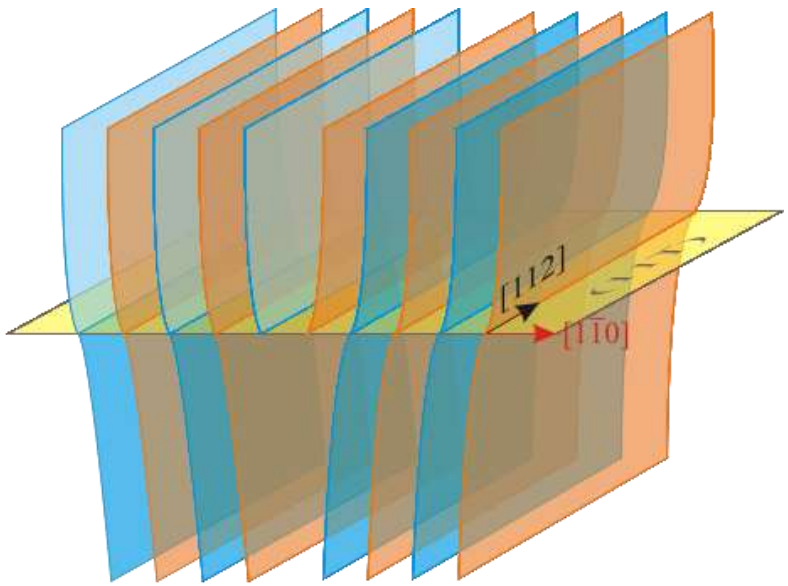


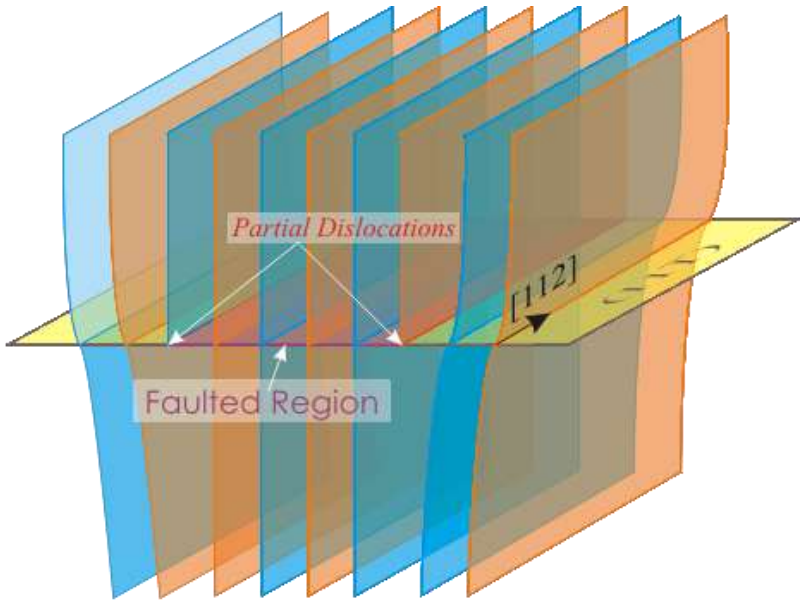
Crystal dislocations: FCC structure



Energy of the perfect dislocation $= G \cdot b^2 = G \cdot (a/2<110>)^2 = \frac{G \cdot a^2}{2}$

Energy of the two partial dislocations $= 2G \cdot (a/6<112>)^2 = 2G \cdot a^2/36 \cdot (1^2 + 1^2 + 2^2) = \frac{G \cdot a^2}{3}$





Introduction: dependence of deformation on SFE

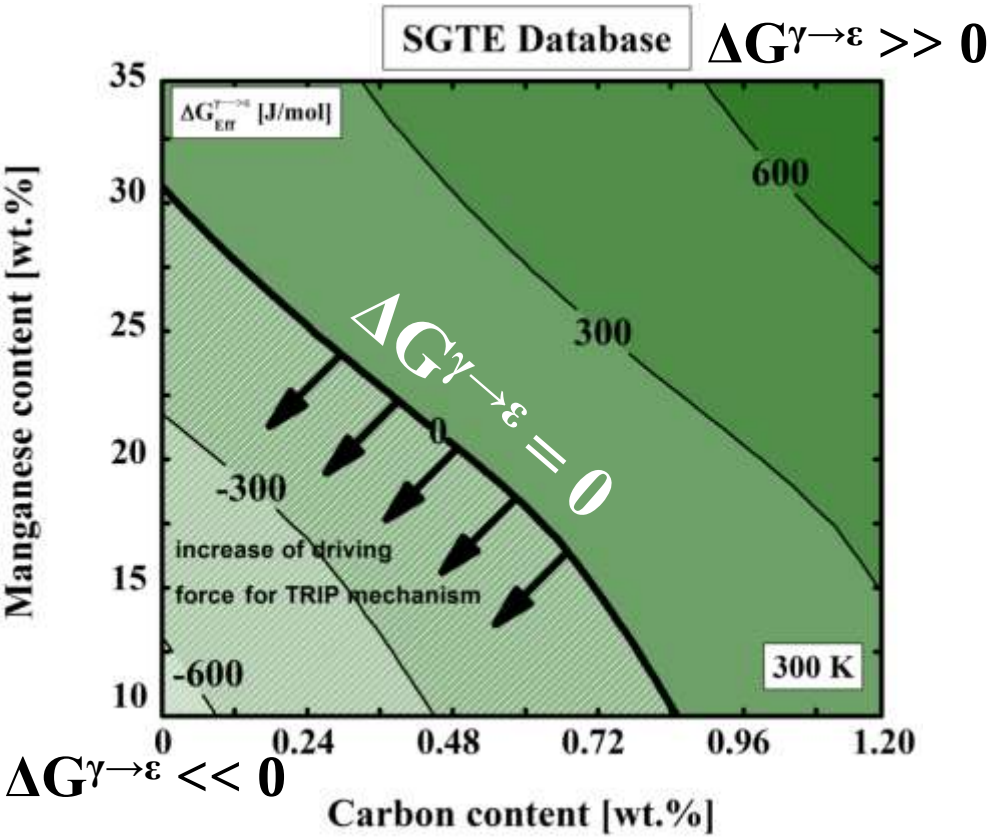
lower SFE →

γ (fcc) cells → γ (fcc) planar → γ (fcc+kappa) planar → γ (fcc+twins) → ε (hcp) → α' (bcc/bct)

high-Mn+Al

high-Mn (15-30%)

medium-Mn (5-12%)



Critical stress for twin growth:

$$\tau_c = \frac{\gamma_{sf}}{3b_s} + \frac{3Gb_s}{L_0}$$

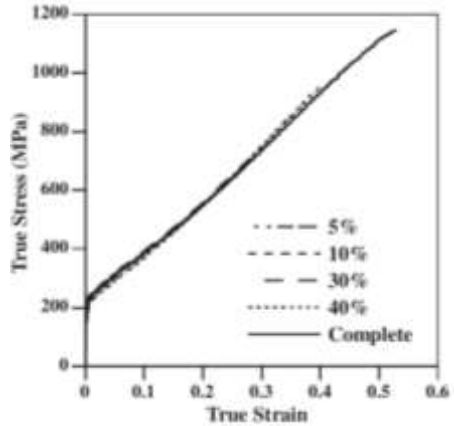
Critical stress for ε-martensite growth:

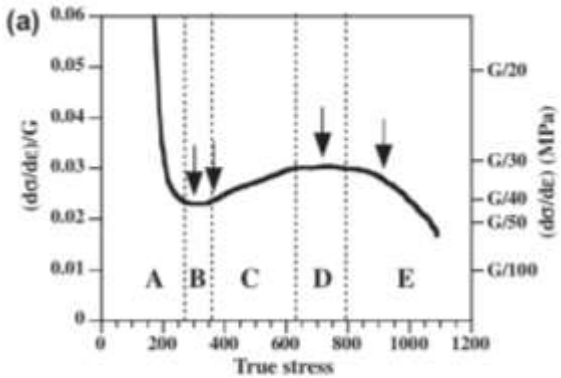
$$\tau_c = \frac{\gamma_{sf}}{3b_s} + \frac{3Gb_s}{L_0} + \frac{h\Delta G^{\gamma\to\varepsilon}}{3b_s}$$

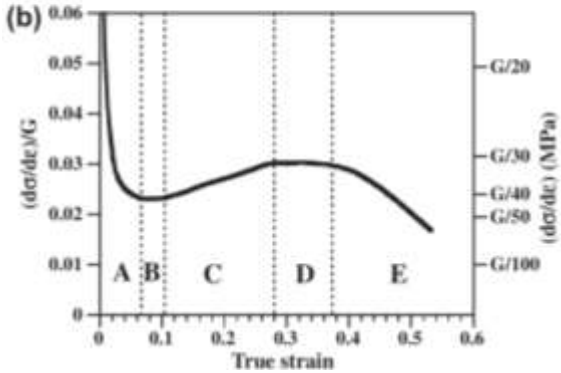
Outline: High Mn steels

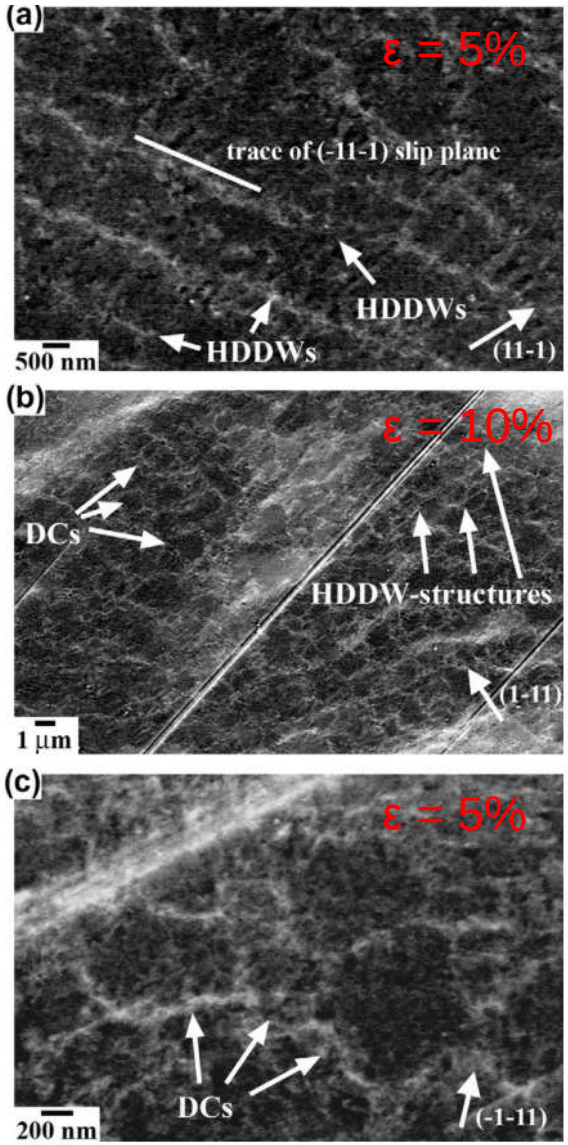
1. High-Mn TWIP steels
2. Weight reduced high Mn – high Al steels – as quenched
3. Weight reduced high Mn – high Al steels – kappa carbides

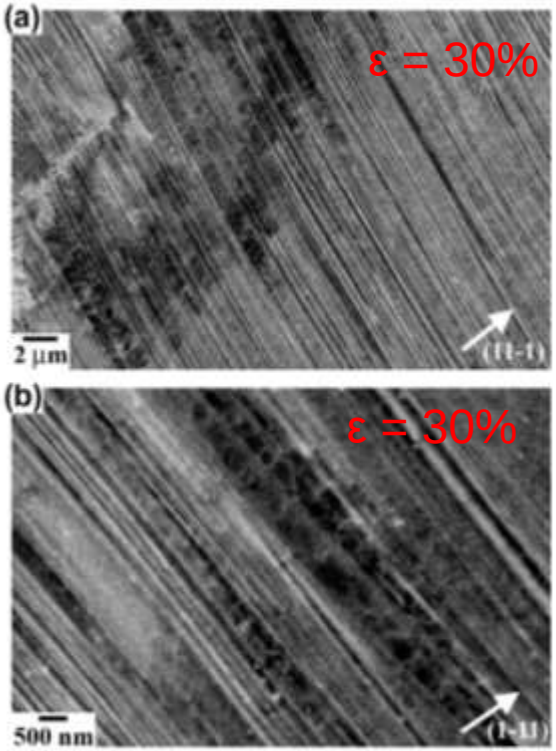
Fe-22Mn-0.6C TWIP steel (wt.%)









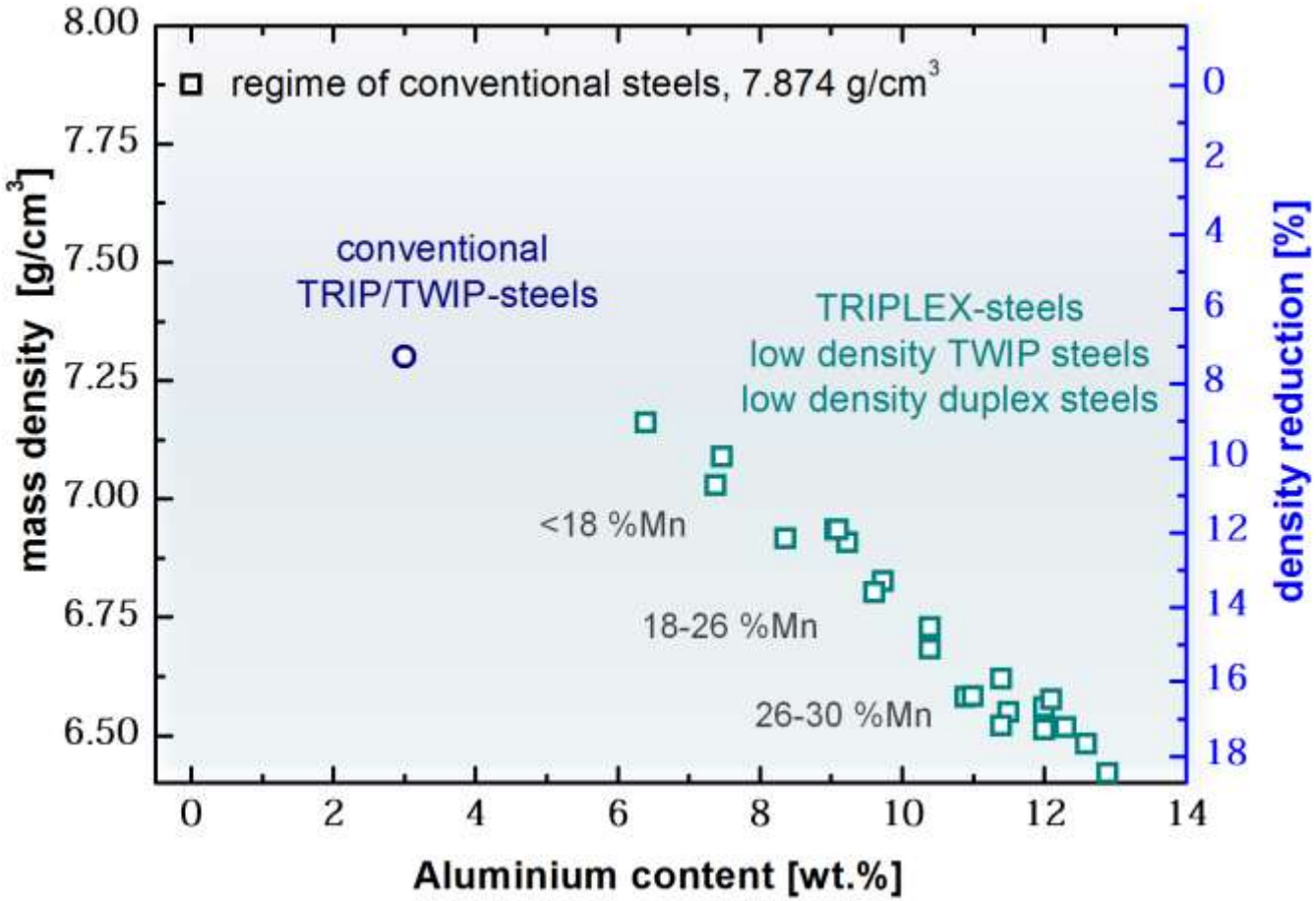


Gutierrez-Urrutia et al. (2012) Acta Mater. 60, p. 5791, Gutierrez-Urrutia et al. (2011) Acta Mater. 59, p. 6449

Outline: High Mn steels

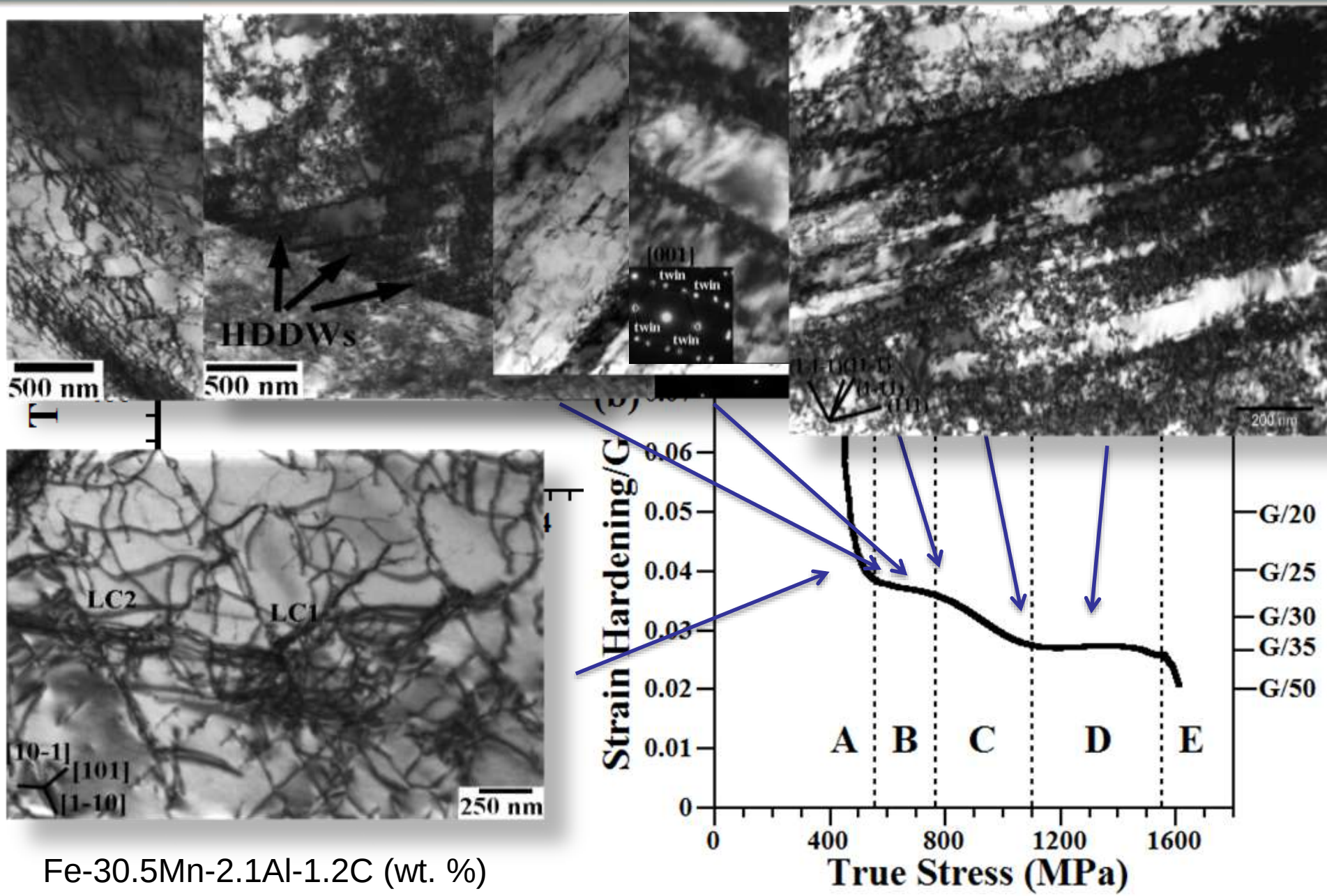
1. High-Mn TWIP steels
2. Weight reduced high Mn – high Al steels – as quenched
3. Weight reduced high Mn – high Al steels – kappa carbides

Fe-30%Mn-8%Al-1.2%C – 10-18% Weight reduction



Raabe et al (2015) Steel Research International, 86 (10), pp. 1127

Rapid alloy prototyping: Fe-Mn-Al-C steels: not heat treated

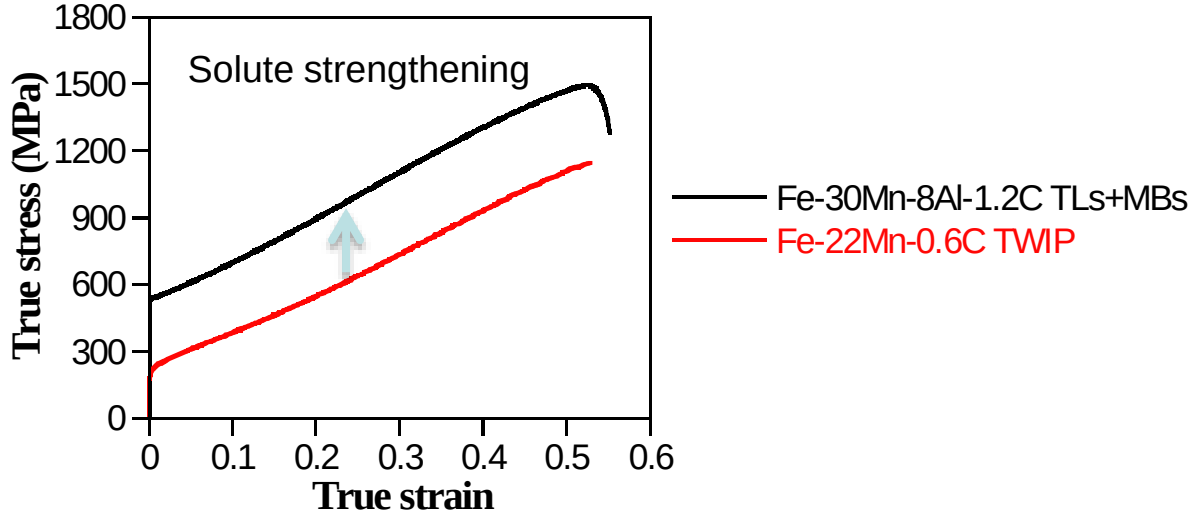


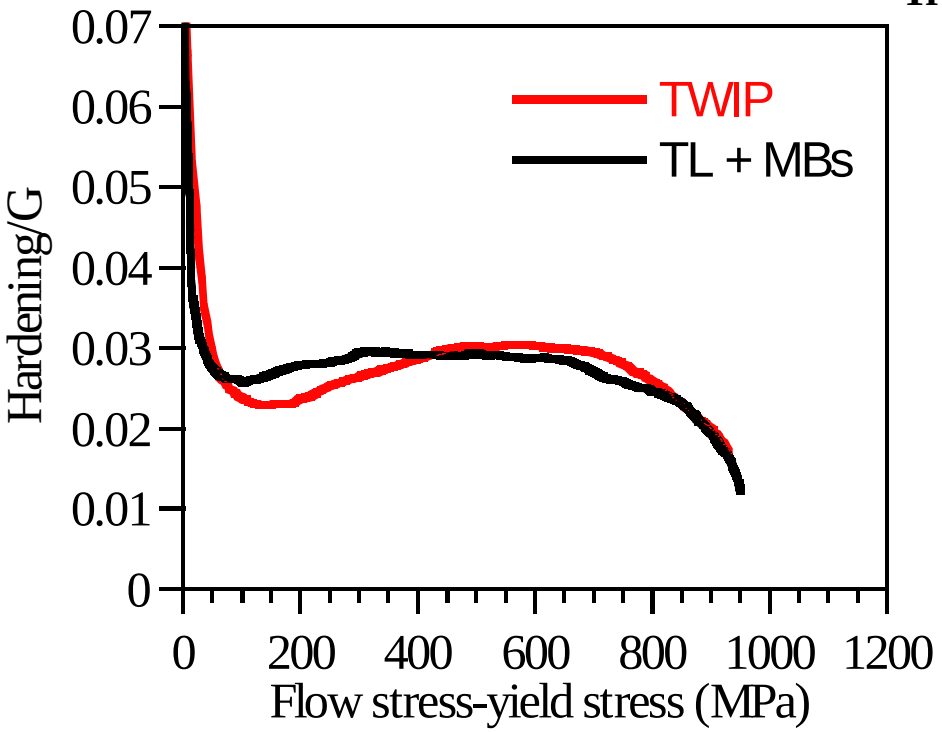
Fe-30.5Mn-2.1Al-1.2C (wt. %)

Gutierrez-Urrutia, et al . Acta Materialia 60 (2012) 5791

Fe-30Mn-8Al-1.2C (wt%), as-quenched, no kappa precipitates

Solid solution
Dynamic microband refinement



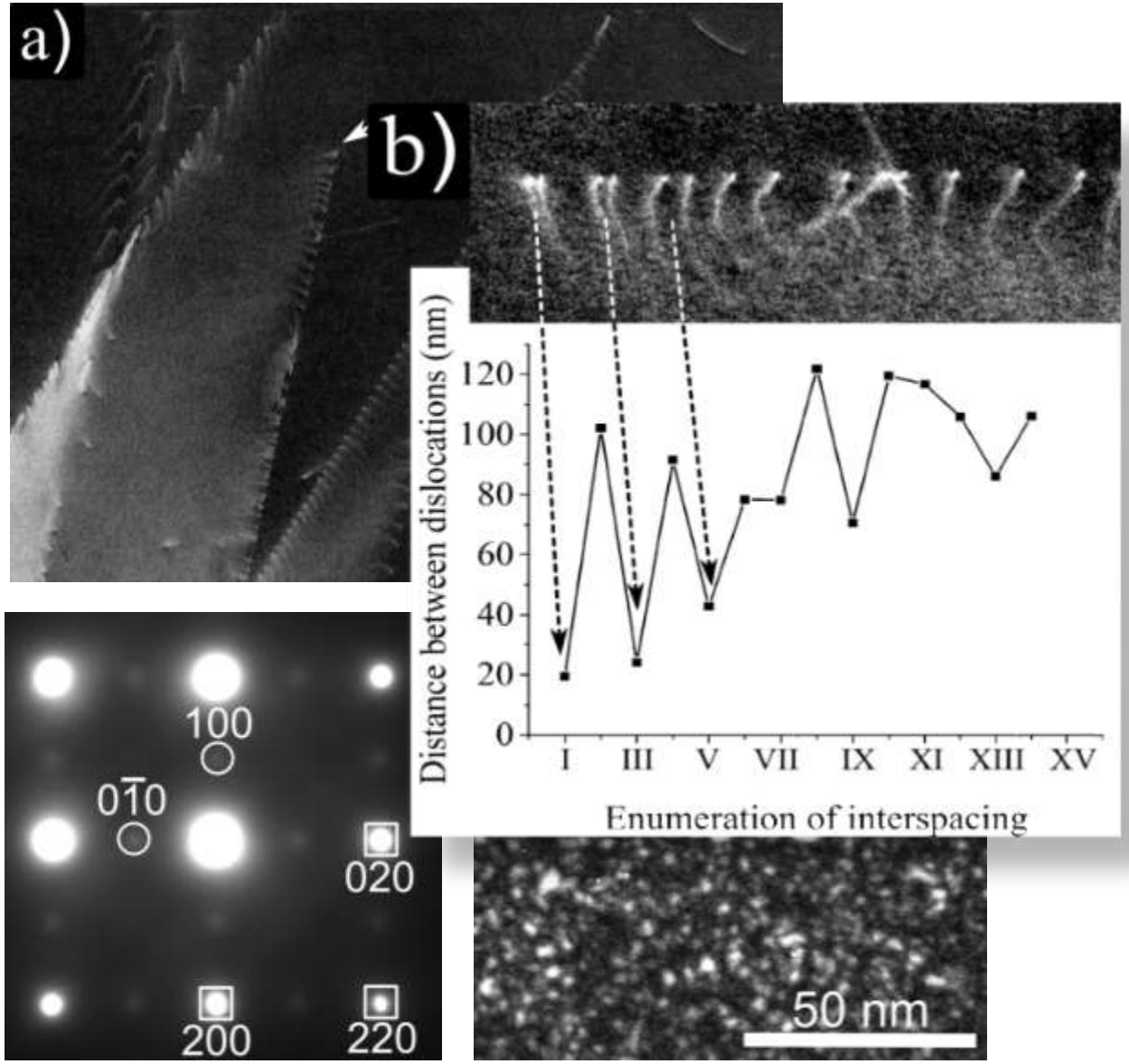


TLs: Taylor lattices
MBs: Microbands

Similar strain hardening

Fe-30.4Mn-8Al-1.2C (wt%), as-quenched, no kappa precipitates

Electron Channeling Contrast Imaging ECCI



Welsch et al. (2016) Acta Materialia, 116, pp. 188

Outline: High Mn steels

1. High-Mn TWIP steels
2. Weight reduced high Mn – high Al steels – as quenched
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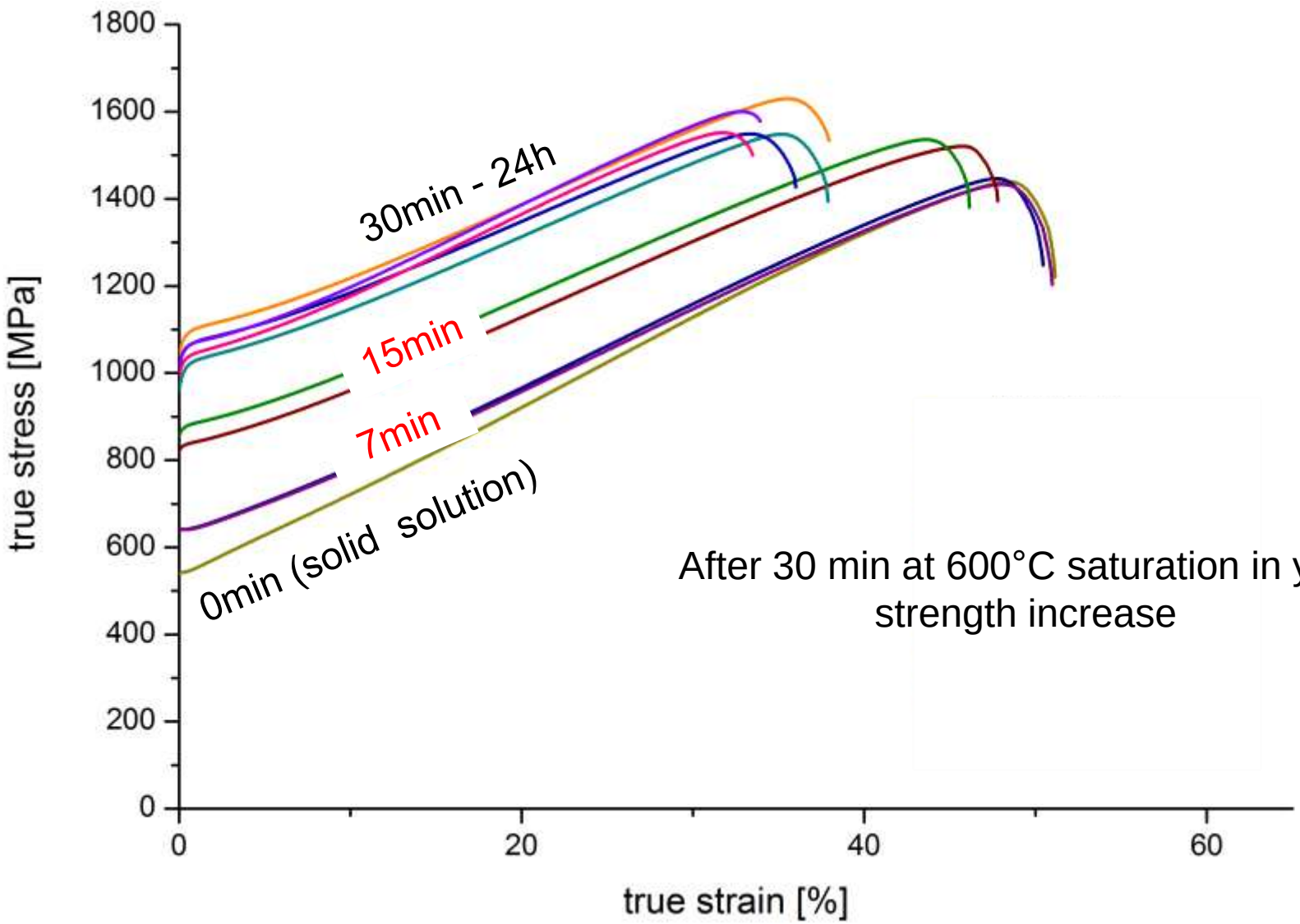
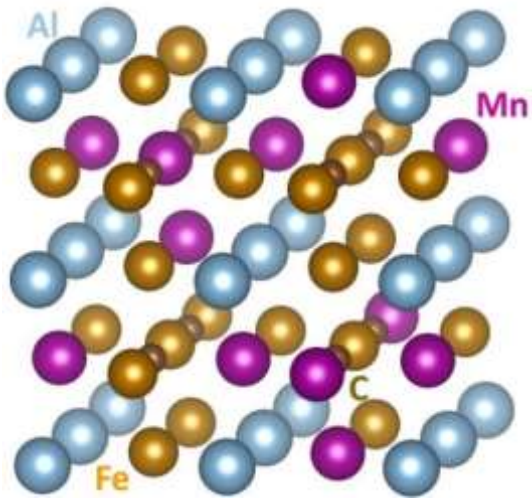
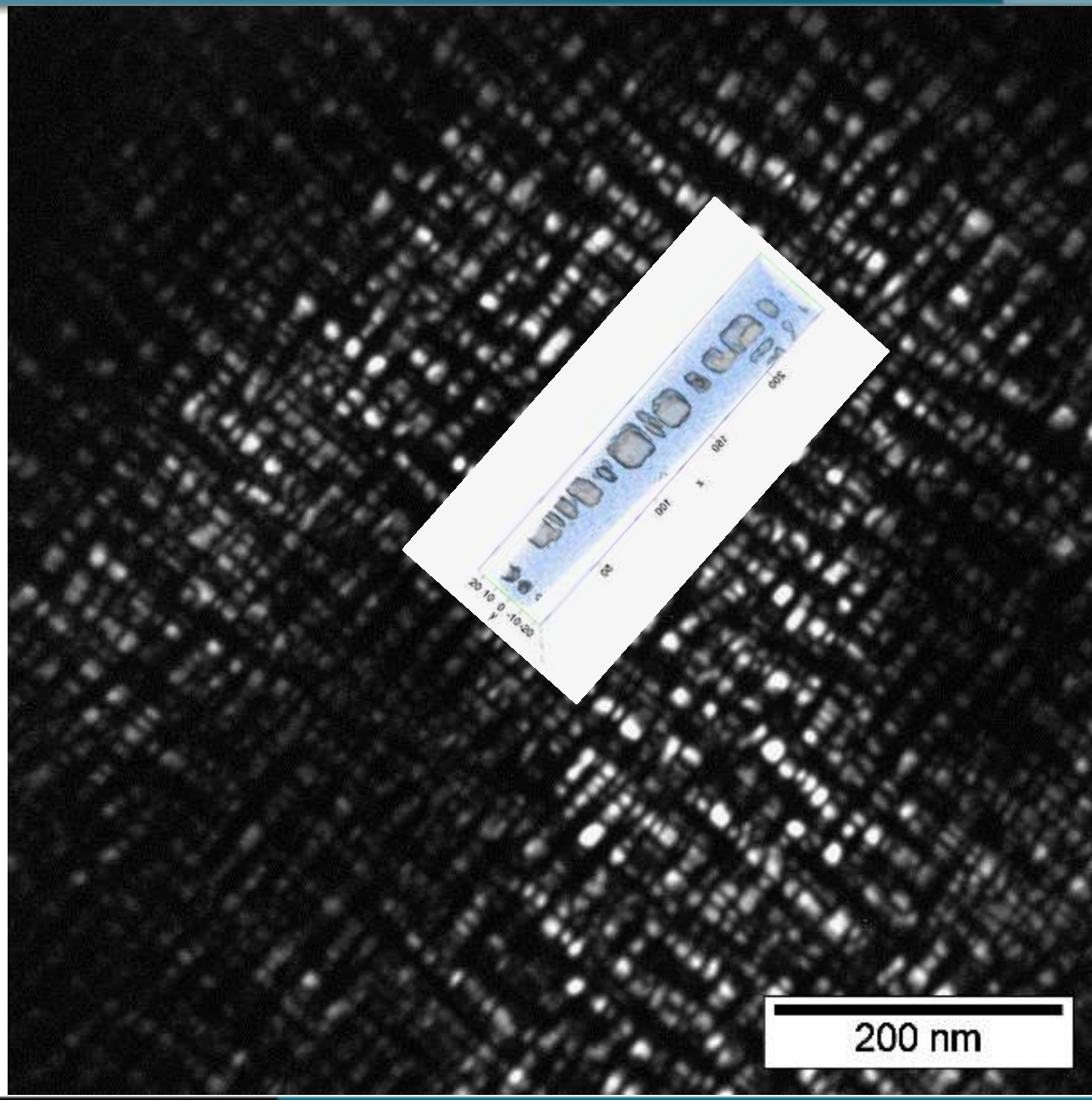
Fe-30Mn-8Al-1.2C, different annealing times at 600°C



After 30 min at 600°C saturation in yield strength increase

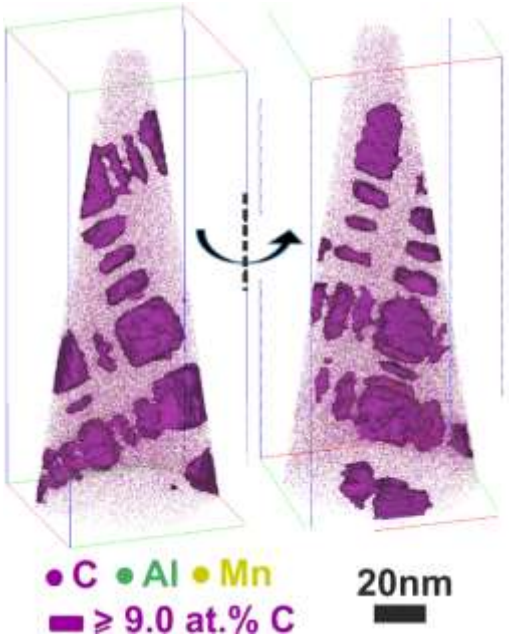
Fe-30%Mn-7.7%Al-1.3%C (wt.%) – 10-18% weight reduction

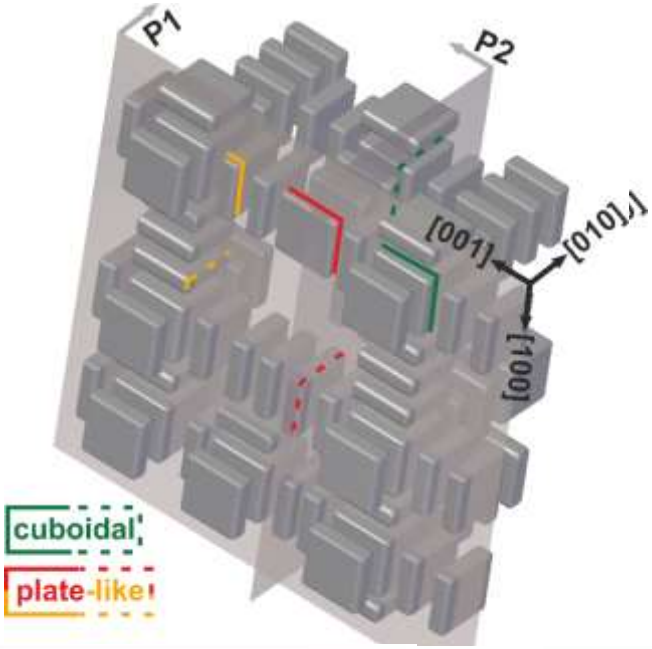


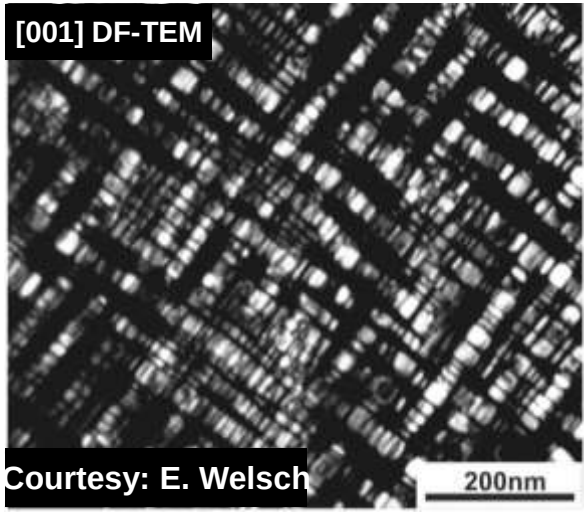


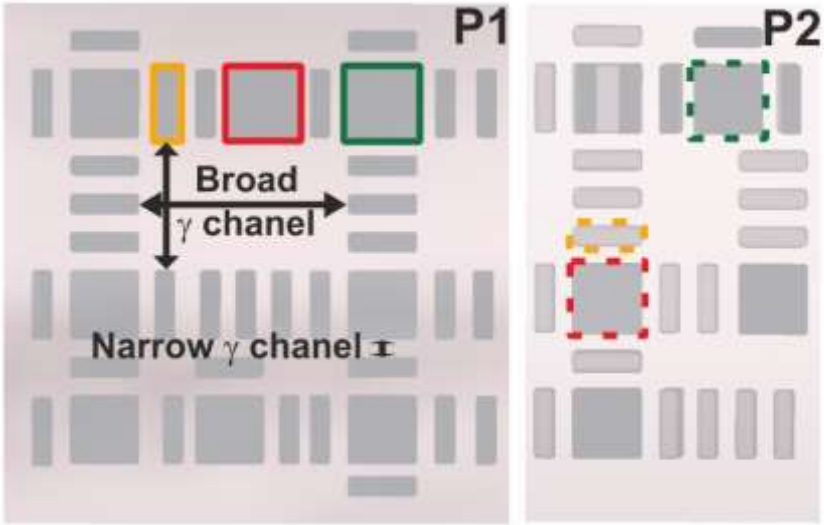
Yao, M.J. et al. Acta Materialia 106 (2016) 229

600°C-24h-aged: kappa particle morphology

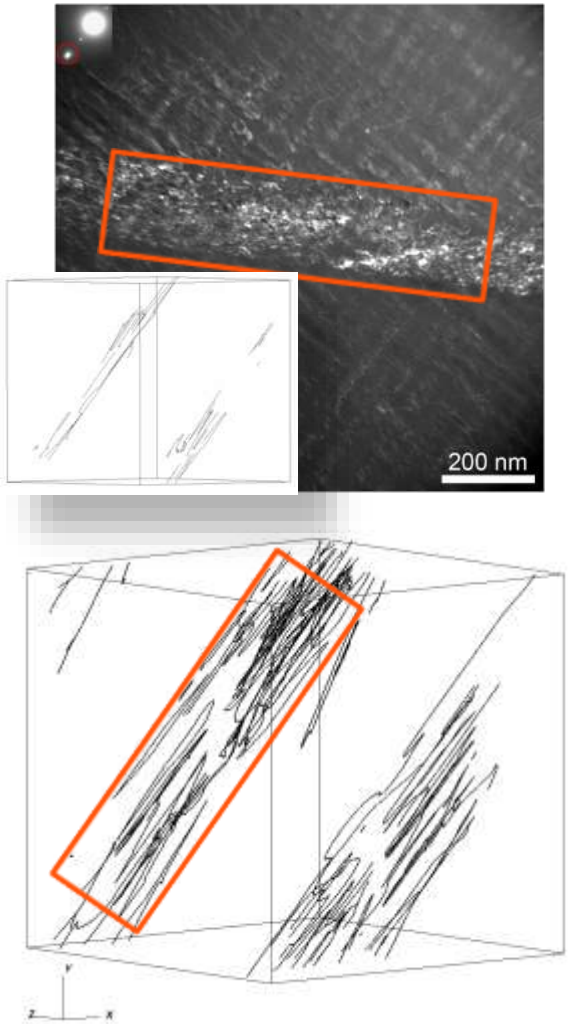




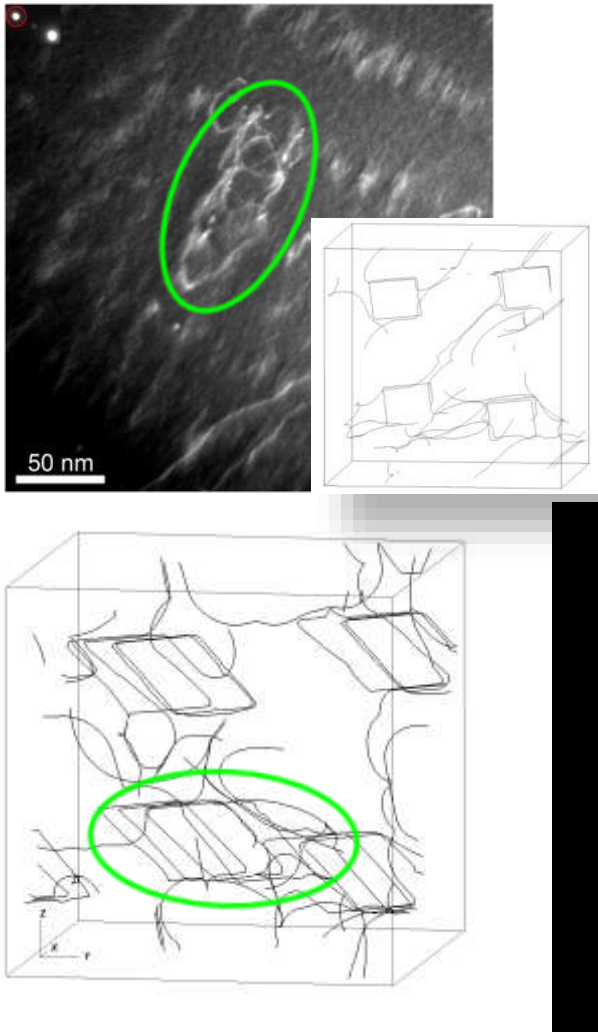




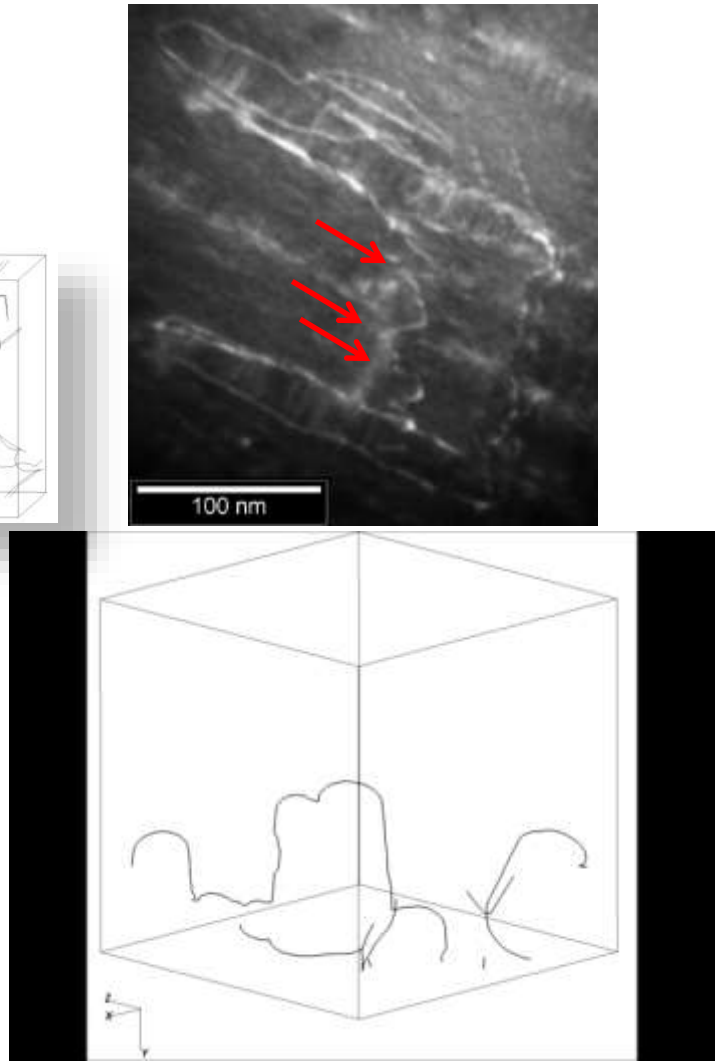
Analyzing microstructure features using DDD



Formation of slip bands from individual dislocation sources

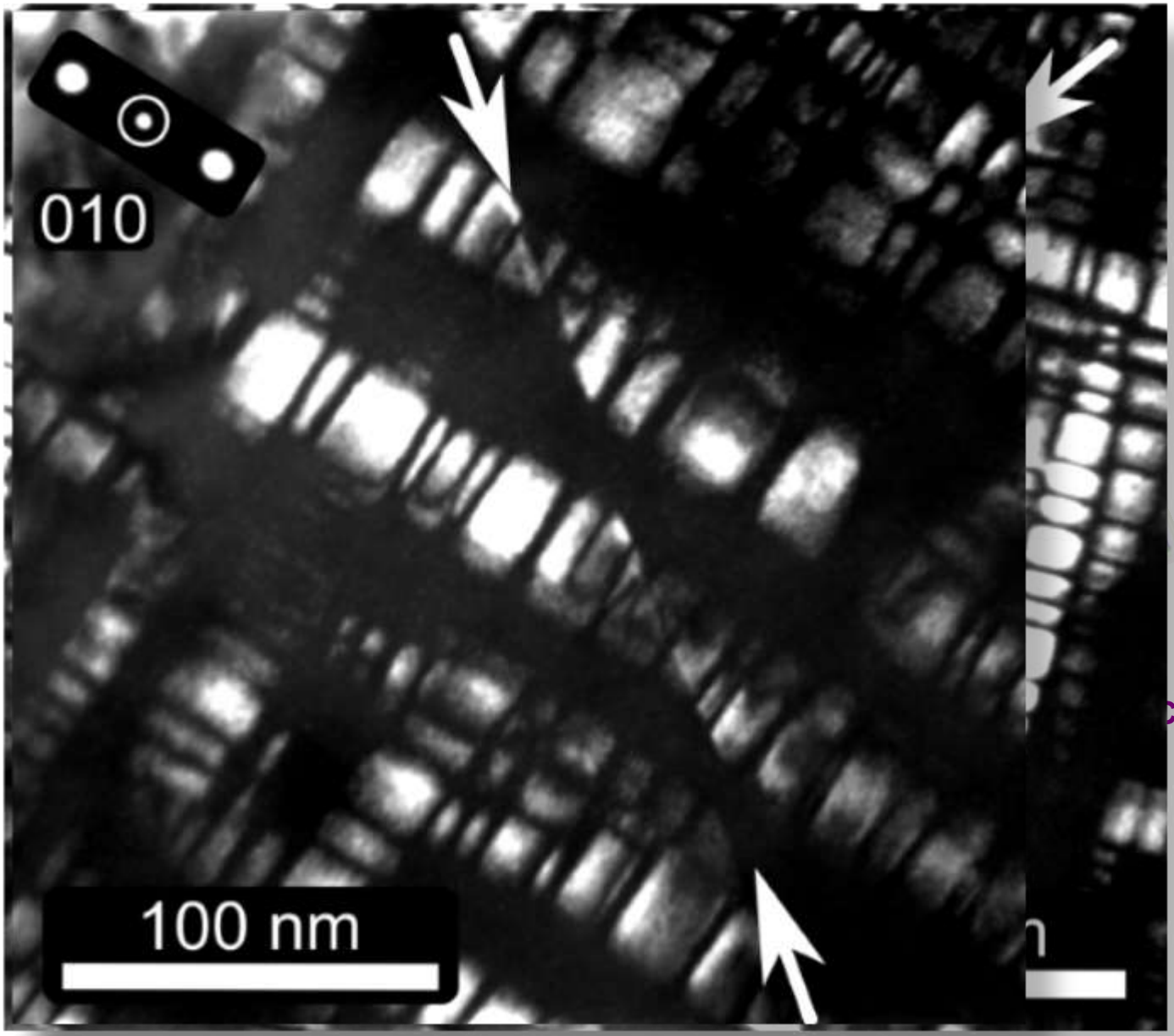


Dislocation wrapping around κ-carbides



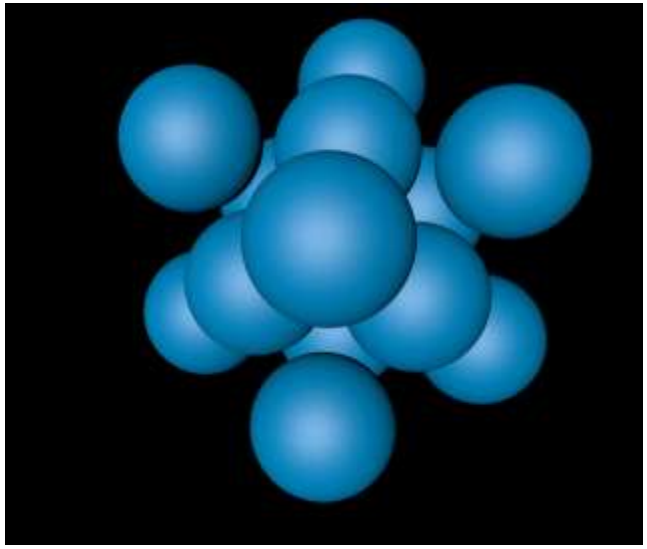
Dislocation pinning due to cross-slip into different conjugate glide plane

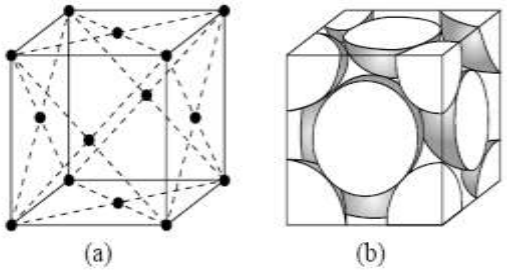
8Al-600°C-24h-aged, ε=15%, correlative TEM-APT

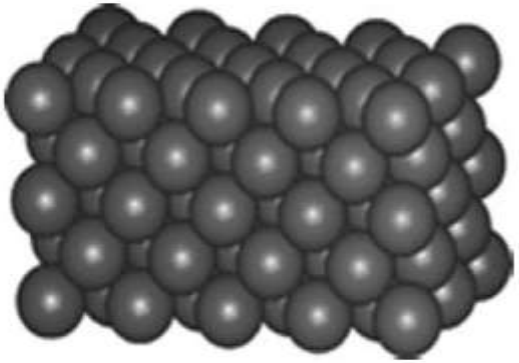


Crystal structure: FCC

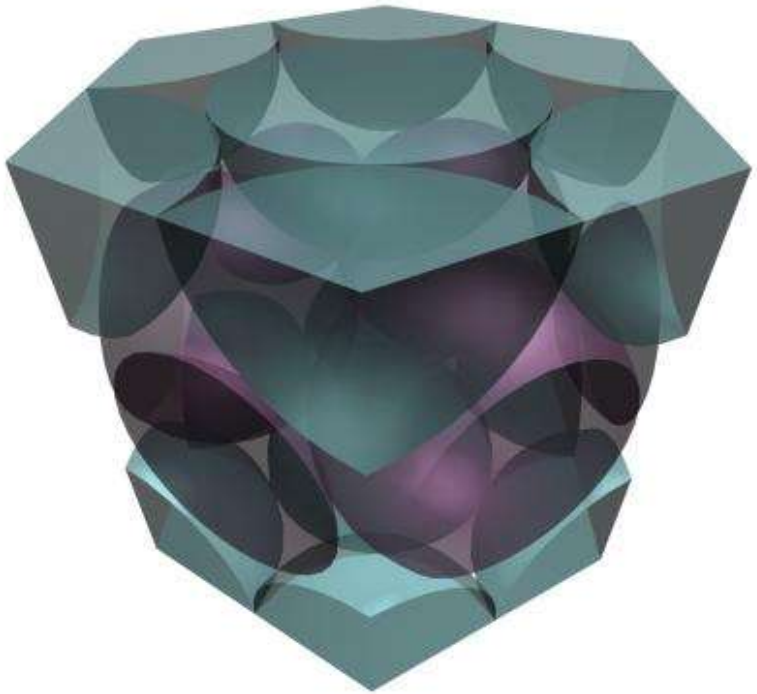
Fe (γ), Al, Cu, Au





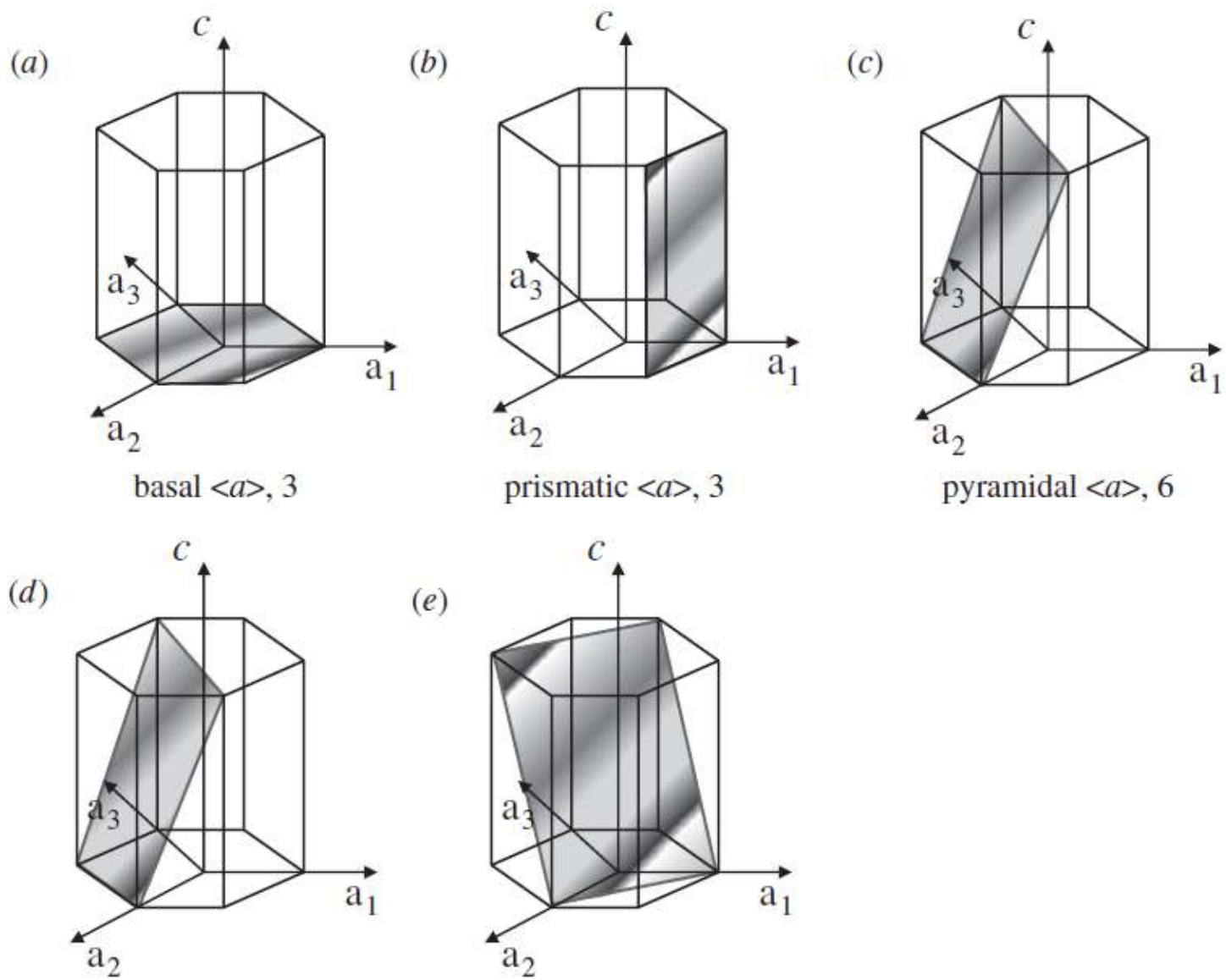


Crystal structure: Hexagonal



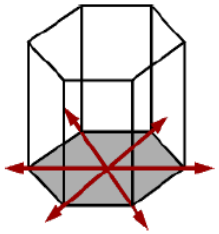
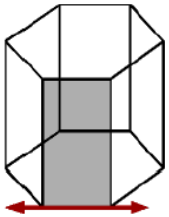
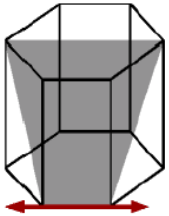
Seperate class by Dr. Sandlöbes

Crystal structure: Hexagonal



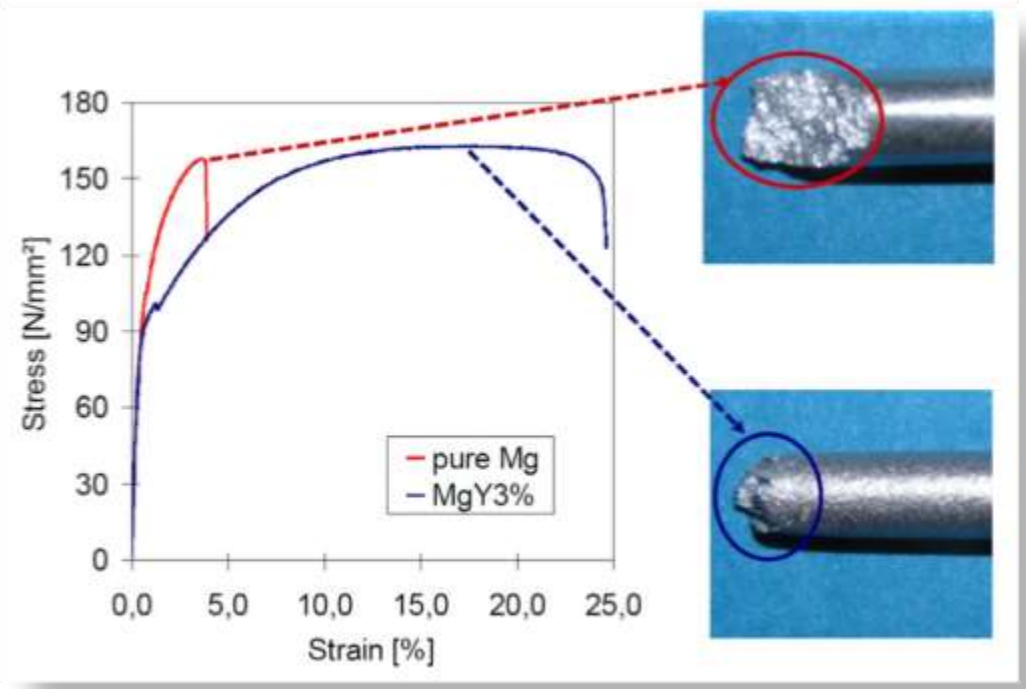
Miller Indices

vectors and planes for hexagonal materials

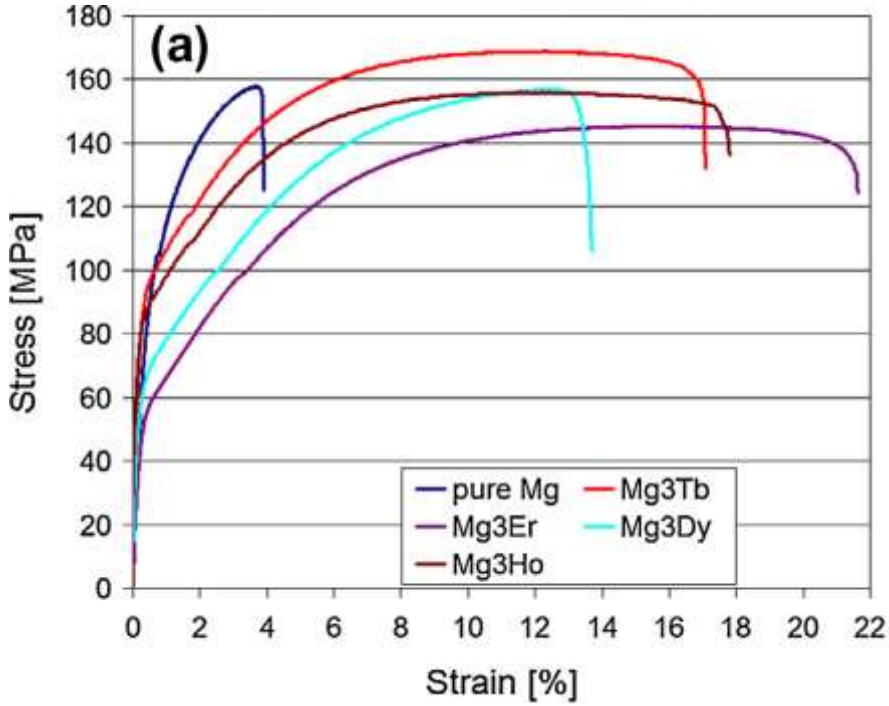
Gitter	Beispiel		Gleitebenen G		Gleitrichtung g		Gesamtzahl der Gleitsysteme
			Typ	Zahl	Typ	Zahl	
hex	Cd Zn Mg Ti_α Be		(0001)	1	[1120]	3	3
	Cd Zn Mg Ti_α Be Zr_α		(1010)	3	[1120]	1	3
	Mg Ti_α		(1011)	6	[1120]	1	6

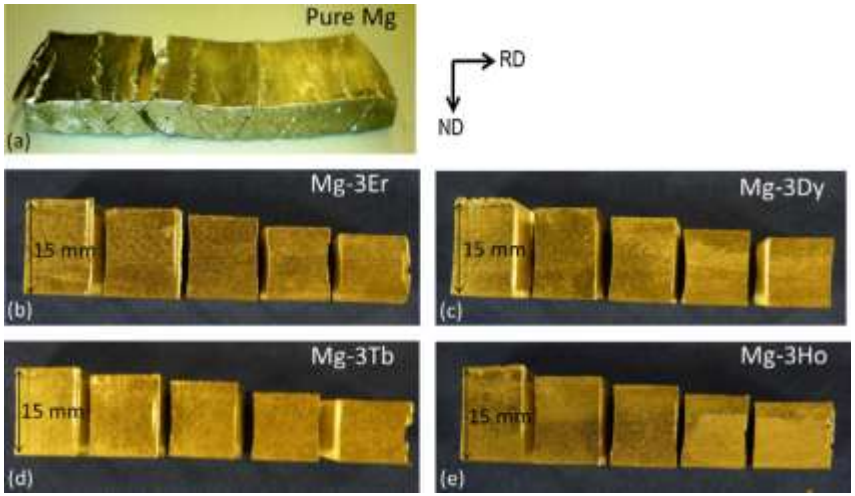
hexagonal alloy systems: crystal structure and plasticity: examples

Mg - RE



Crystal dislocations: Hex structure – example of Mg





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Microstructure Mechanics

Dislocation statics

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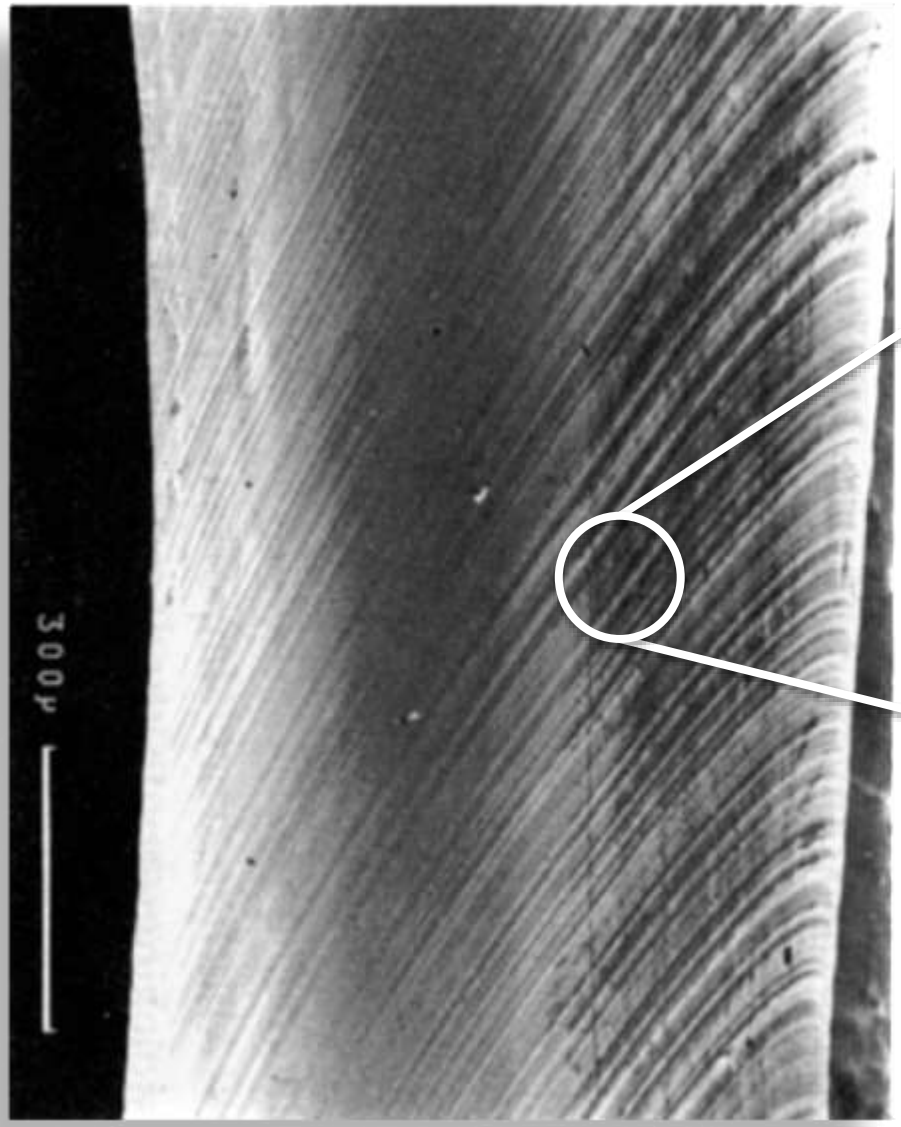
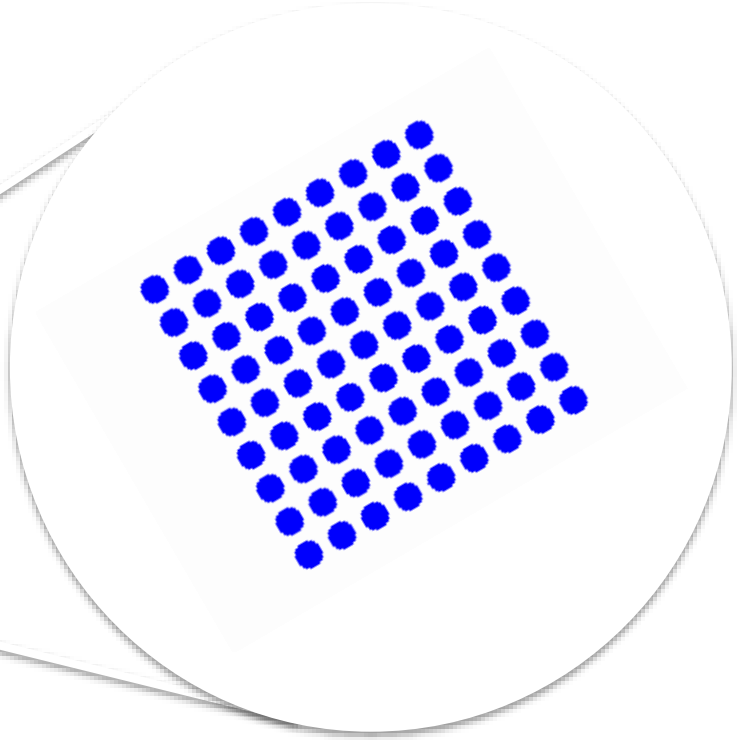
Plastic deformation of a single crystal by dislocation slip

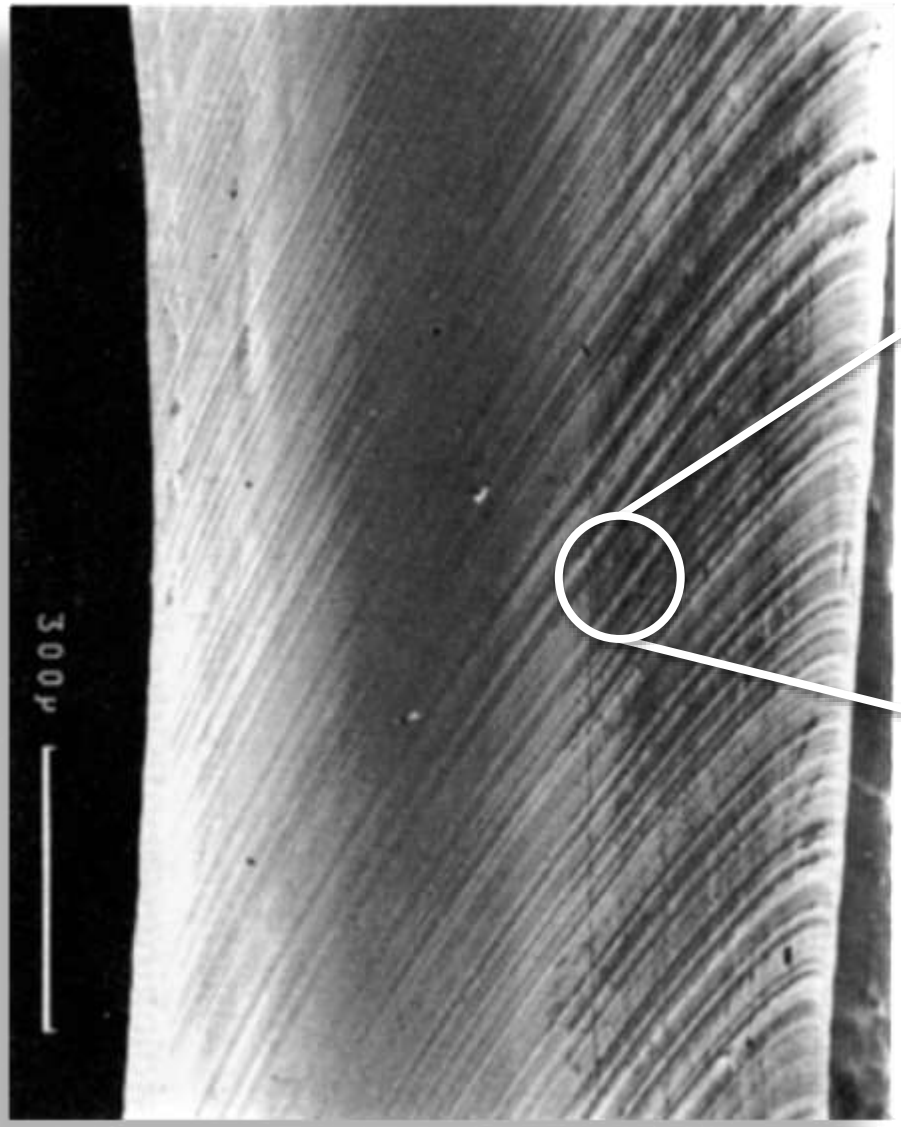


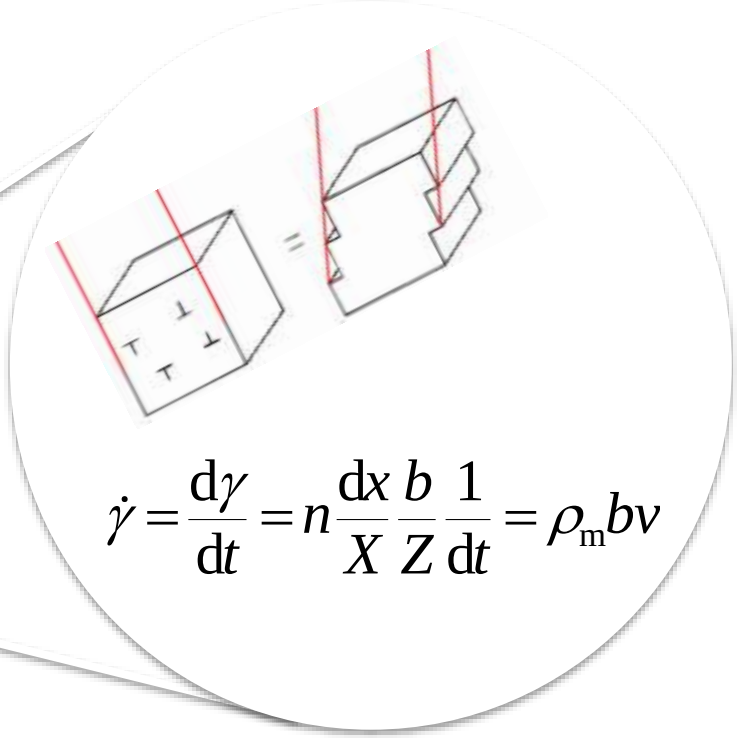
single slip in a single crystal



plastic anisotropy

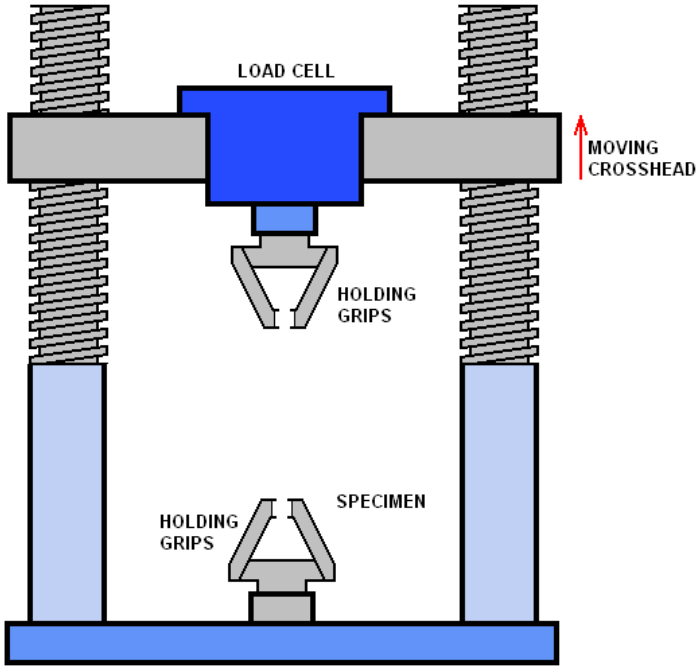
Plastic deformation of a single crystal by dislocation slip

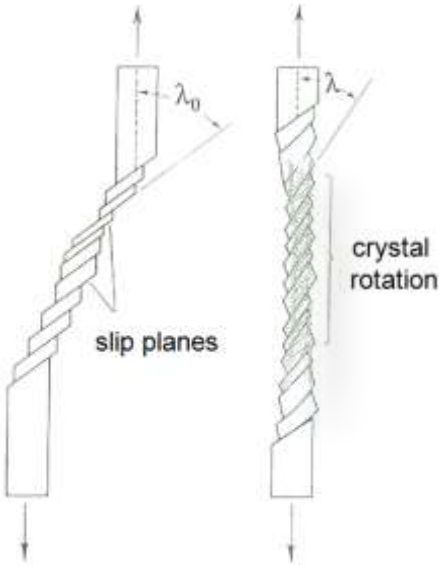




$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

Boundary condition: determines lab frame constraints





Constraints lead to specific crystal rotations

Non-symmetric dislocation shear leads to rotation

Symmetric-shear can lead to shape change without rotation

Change in local constraints leads to heterogeneity

Roters et al. Acta Mater.58 (2010)

Kinematics: displacement vector in continuum space

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

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

Kinematics: displacement vector in continuum space

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

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

Kinematics, displacement, displacement gradient: general

Distorsions come from gradients in the displacement fields

Displacement vector:

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

Strain tensor:

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

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

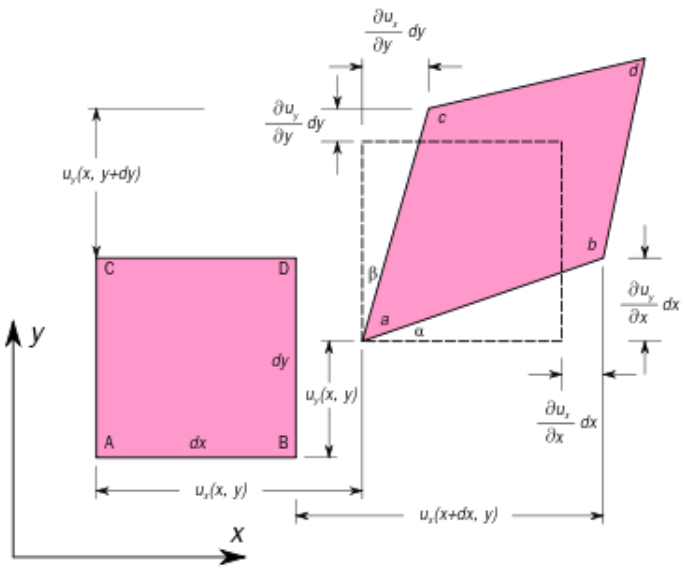
etc.

Strain tensor: symmetrical part of displacement gradient tensor

Displacement gradient

The tensor $\frac{\partial u_i}{\partial x_j}$ is called **displacement gradient tensor** and may be written as

$$\frac{\partial u_i}{\partial x_j} = u_{i,j} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix}$$



Displacement gradient tensor

The displacement gradient tensor in general is a non-symmetric tensor and can be decomposed into symmetric and antisymmetric part. Hence the displacement is

$$u_i = \underbrace{u_i^0}_{\text{translation vector}} + \underbrace{\frac{1}{2}\left(u_{i,j} + u_{j,i}\right)}_{\text{strain tensor}} \mathrm{d}x_j + \underbrace{\frac{1}{2}\left(u_{i,j} - u_{j,i}\right)}_{\text{rotation tensor}} \mathrm{d}x_j$$

$$= u_i^0 + \varepsilon_{ij}\mathrm{d}x_j + \omega_{ij}\mathrm{d}x_j$$

Displacement gradient tensor: the Cauchy strain

Strain tensor

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$$

In matrix form

$$\varepsilon = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)$$

The above strain tensor is called **Caushy strain tensor**

Displacement gradient tensor: the Cauchy strain

$$
\begin{aligned}
\varepsilon_{ij} &= \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \\
&= \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\partial u1}{\partial x1} & \frac{1}{2}\left(\frac{\partial u1}{\partial x2} + \frac{\partial u2}{\partial x1}\right) & \frac{1}{2}\left(\frac{\partial u1}{\partial x3} + \frac{\partial u3}{\partial x1}\right) \\ \frac{1}{2}\left(\frac{\partial u2}{\partial x1} + \frac{\partial u1}{\partial x2}\right) & \frac{\partial u2}{\partial x2} & \frac{1}{2}\left(\frac{\partial u2}{\partial x3} + \frac{\partial u3}{\partial x2}\right) \\ \frac{1}{2}\left(\frac{\partial u3}{\partial x1} + \frac{\partial u1}{\partial x3}\right) & \frac{1}{2}\left(\frac{\partial u3}{\partial x2} + \frac{\partial u2}{\partial x3}\right) & \frac{\partial u3}{\partial x3} \end{bmatrix}
\end{aligned}
$$

Displacement gradient tensor: the rotation

Rotation tensor

$$\omega_{ij} = \frac{1}{2}\left(u_{i,j} - u_{j,i}\right)$$

In matrix form

$$\omega = \frac{1}{2}\left(\nabla\mathbf{u} - (\nabla\mathbf{u})^T\right)$$

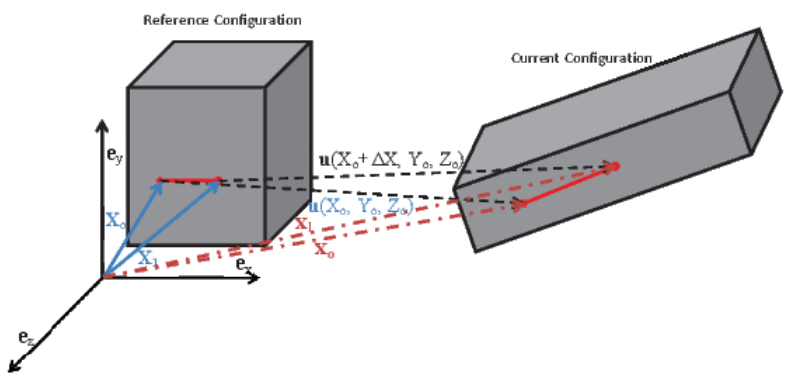
Displacement gradient tensor

Matrix expression of the strain tensor

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_{zz} \end{bmatrix}$$

Matrix expression of the rotation tensor

$$\omega = \begin{bmatrix} 0 & \omega_{xy} & \omega_{xz} \\ -\omega_{xy} & 0 & \omega_{yz} \\ -\omega_{xz} & -\omega_{yz} & 0 \end{bmatrix}$$



Displacement gradient tensor: strain components

Normal strains

$$\varepsilon_{xx} = \frac{\partial u}{\partial x}, \quad \varepsilon_{yy} = \frac{\partial v}{\partial y}, \quad \varepsilon_{zz} = \frac{\partial w}{\partial z}$$

Shear strains

$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

$$\varepsilon_{xz} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)$$

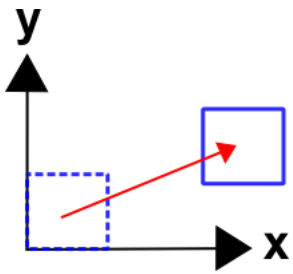
$$\varepsilon_{yz} = \frac{1}{2}\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)$$

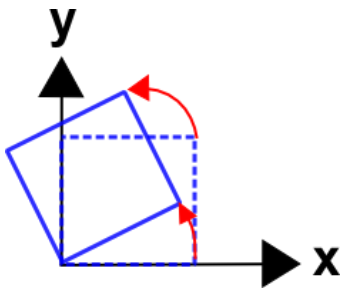
Engineering shear strains

$$\gamma_{xy} = 2\varepsilon_{xy}, \quad \gamma_{xz} = 2\varepsilon_{xz}, \quad \gamma_{yz} = 2\varepsilon_{yz}$$

Displacement gradient tensor: special cases

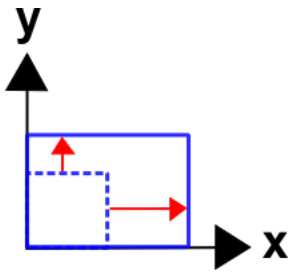
Rigid Body Displacements

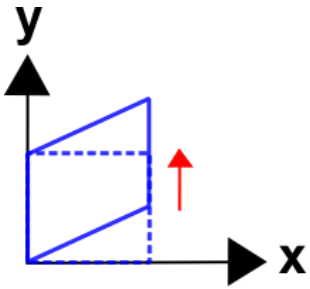




Rigid Body Rotations

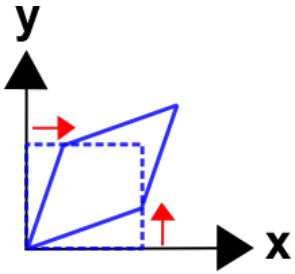
Stretching



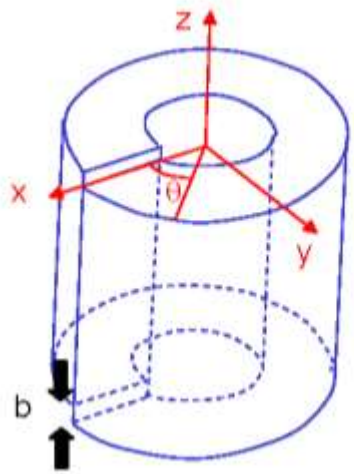


Shear (with Rotation)

Pure Shear



Displacement and strain field: infinite straight screw dislocation



"Recipe" :
- take a hollow cylinder, axis along z:
- cut on a plane parallel to the z-axis;
-displace the free surfaces by **b** in the z-direction.

By inspection:

$$u_x = u_y = 0$$

$$u_z = \frac{b\theta}{2\pi} = \frac{b}{2\pi}\tan^{-1}\left(\frac{y}{x}\right)$$

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0$$

$$\varepsilon_{xz} = \tfrac{1}{2}\frac{\partial u_z}{\partial x} = \frac{b}{4\pi}\frac{\partial}{\partial x}\tan^{-1}\left(\frac{y}{x}\right) = -\frac{b}{4\pi}\frac{1}{1+\left(y/x\right)^2}\frac{y}{x^2} = -\frac{b}{4\pi}\frac{y}{x^2+y^2} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\varepsilon_{yz} = \tfrac{1}{2}\frac{\partial u_z}{\partial y} = \frac{b}{4\pi}\frac{\partial}{\partial y}\tan^{-1}\left(\frac{y}{x}\right) = \frac{b}{4\pi}\frac{1}{1+\left(y/x\right)^2}\frac{1}{x} = \frac{b}{4\pi}\frac{x}{x^2+y^2} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

Stress field of straight screw dislocation

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0$$

$$\varepsilon_{xz} = -\frac{b}{4\pi}\frac{y}{x^2+y^2} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\varepsilon_{yz} = \frac{b}{4\pi}\frac{x}{x^2+y^2} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0$$

$$\Delta = 0$$

$$\sigma_{xz} = 2G\varepsilon_{xz} = -\frac{Gb}{2\pi}\frac{y}{x^2+y^2} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = 2G\varepsilon_{yz} = \frac{Gb}{2\pi}\frac{x}{x^2+y^2} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

In Polar coordinates:

(either by direct inspection, or by transforming the strains and stresses from Cartesian co-ordinates)

$$\varepsilon_{\theta z} = \varepsilon_{z\theta} = \frac{b}{4\pi r}$$

$$\sigma_{\theta z} = \sigma_{z\theta} = \frac{Gb}{2\pi r}$$

All other components of the stress tensor are zero.

Note:
- Stress and strain fields are pure shear
- Fields have radial symmetry
- Stresses and strains are proportional to 1/r:
  - extend to infinity
  - tend to infinite values as $r \Rightarrow 0$

Infinite stresses cannot exist in real materials: the dislocation core radius r_0 is that within which our assumption of linear elastic behaviour breaks down. Typically $r_0 \approx 1$ nm.

Summary: infinite straight screw dislocation

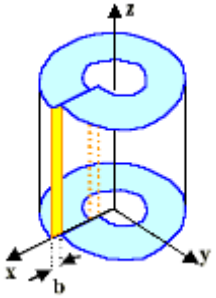
$$\underline{u}(\underline{x}) = \begin{pmatrix} 0 \\ 0 \\ \frac{b}{2\pi} \arctan \frac{y}{x} \end{pmatrix}$$

$$\underline{\underline{\varepsilon}}(\underline{x}) = \begin{pmatrix} 0 & 0 & -\frac{b}{4\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{b}{4\pi}\frac{x}{x^2+y^2} \\ -\frac{b}{4\pi}\frac{y}{x^2+y^2} & \frac{b}{4\pi}\frac{x}{x^2+y^2} & 0 \end{pmatrix}$$

$$\underline{\underline{\sigma}}(\underline{x}) = \frac{Gb}{2\pi} \begin{pmatrix} 0 & 0 & -\frac{b}{4\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{b}{4\pi}\frac{x}{x^2+y^2} \\ -\frac{b}{4\pi}\frac{y}{x^2+y^2} & \frac{b}{4\pi}\frac{x}{x^2+y^2} & 0 \end{pmatrix}$$

Summary: infinite straight edge dislocation

$$
\begin{aligned}
u_x &= \frac{b}{2\pi}\left(\arctan\frac{y}{x} + \frac{1}{2(1-\nu)}\frac{xy}{x^2+y^2}\right) \\
u_y &= \frac{b}{2\pi}\left(-\frac{1-2\nu}{2(1-\nu)}\log\sqrt{x^2+y^2} + \frac{1}{2(1-\nu)}\frac{y^2}{x^2+y^2}\right) \\
u_z &= 0
\end{aligned}
$$



$$
\varepsilon_{xx} = \frac{\partial u_x}{\partial x} = \frac{b\,y\,\left((3-2\,\nu)\,x^2 + (1-2\,\nu)\,y^2\right)}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}
$$

$$
\varepsilon_{yy} = \frac{\partial u_y}{\partial y} = \frac{-\left(b\,y\,\left((1+2\,\nu)\,x^2 + (-1+2\,\nu)\,y^2\right)\right)}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}
$$

$$
\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right) = \frac{b\,x\,(-x^2+y^2)}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}
$$

Summary: infinite straight edge dislocation

$$\sigma_{xx} = \frac{b\,G\,y\,\left(3\,x^2 + y^2\right)}{2\,\left(-1+\nu\right)\,\pi\,\left(x^2+y^2\right)^2}$$

$$\sigma_{yy} = \frac{b\,G\,y\,\left(-x^2 + y^2\right)}{2\,\left(-1+\nu\right)\,\pi\,\left(x^2+y^2\right)^2}$$

$$\sigma_{zz} = \frac{b\,G\,\nu\,y}{\left(-1+\nu\right)\,\pi\,\left(x^2+y^2\right)}$$

$$\sigma_{xy} = \frac{b\,G\,x\,\left(-x^2 + y^2\right)}{2\,\left(-1+\nu\right)\,\pi\,\left(x^2+y^2\right)^2}$$

Microstructure Mechanics

Dislocation dynamics

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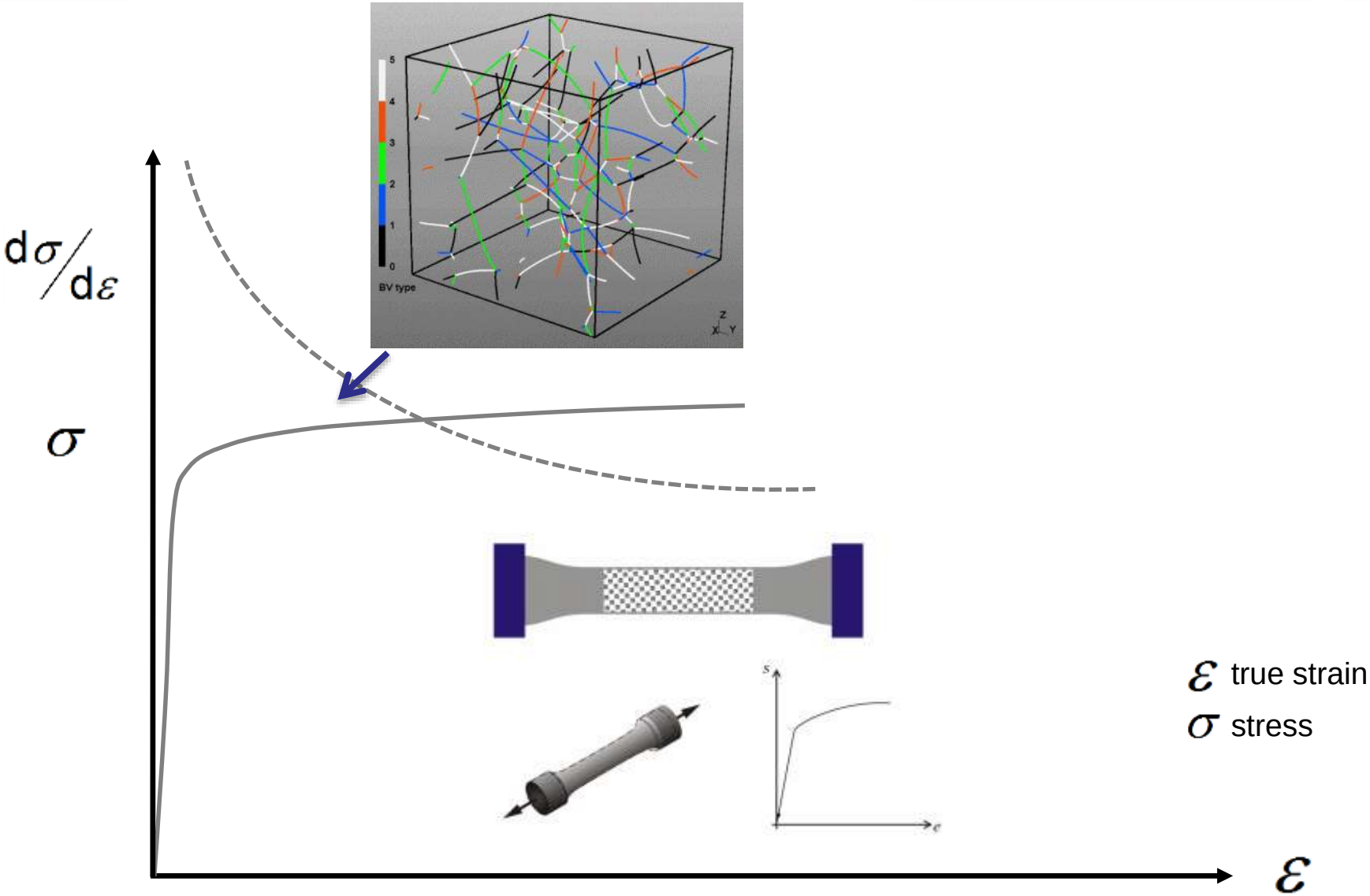
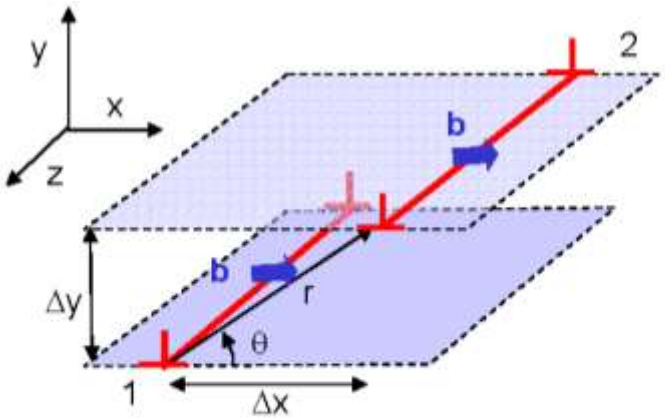
Dislocations and strain hardening



Dynamics: forces among dislocations



Dislocation 2 "feels" the stress field of dislocation 1 (and vice versa).

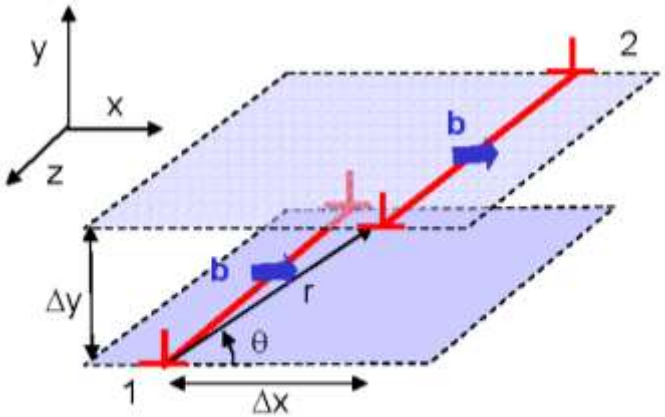
Peach-Koehler Force

$$\vec{F}_{1\to 2} = \left(\underline{\underline{\sigma}}^{1\to 2}\, \vec{b}_2 \right) \times \vec{t}_2$$

σ_{xy} – produces *glide* force

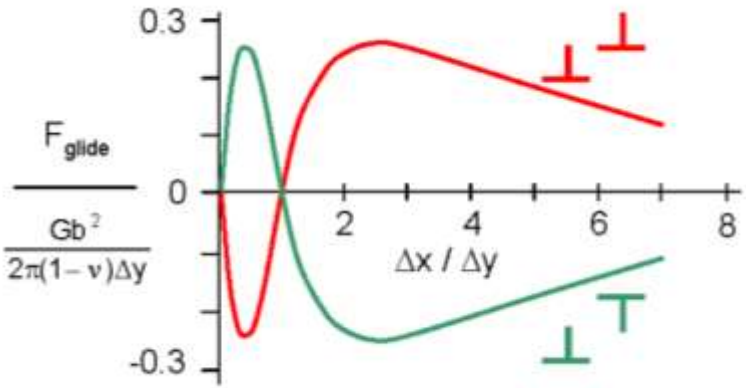
σ_{xx} – produces *climb* force

Forces among edge dislocations



So glide force, resolved onto the slip plane, is:

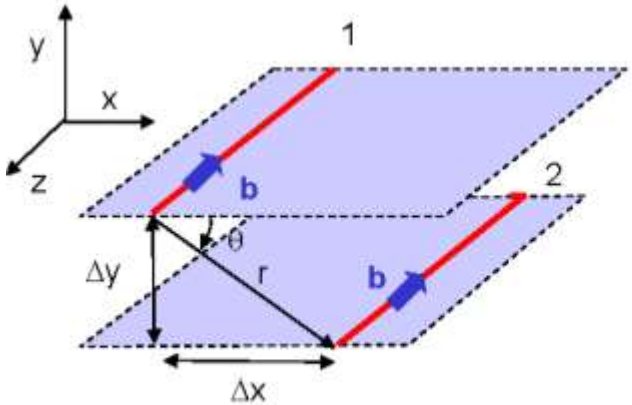
$$F_{glide} = \frac{Gb^2}{2\pi(1-\nu)} \frac{\Delta x(\Delta x^2 - \Delta y^2)}{(\Delta x^2 + \Delta y^2)^2}$$



$$\sigma_{xx} = -D\,y \frac{3\Delta x^2 + \Delta y^2}{(\Delta x^2 + \Delta y^2)^2}, \quad \text{with: } D = \frac{Gb}{2\pi(1-\nu)}$$

$$\sigma_{xy} = \sigma_{yx} = D\,\Delta x \frac{\Delta x^2 - \Delta y^2}{(\Delta x^2 + \Delta y^2)^2}$$

Forces among screw dislocations



Dislocation 2 "feels" the stress field of dislocation 1 (and vice versa).

$$\sigma_{\theta z} = \sigma_{z\theta} = \frac{Gb}{2\pi r}$$

So force on dislocation 2 from dislocation 1 is:

$$F = \frac{Gb^2}{2\pi r}$$

... but this force acts in the radial direction.

Force on dislocation 2 from dislocation 1, resolved onto the glide plane is:

$$F_{res} = \frac{Gb^2}{2\pi r}\cos\theta$$

Alternatively, we can use the stress field expressed in Cartesian co-ordinates:

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0$$

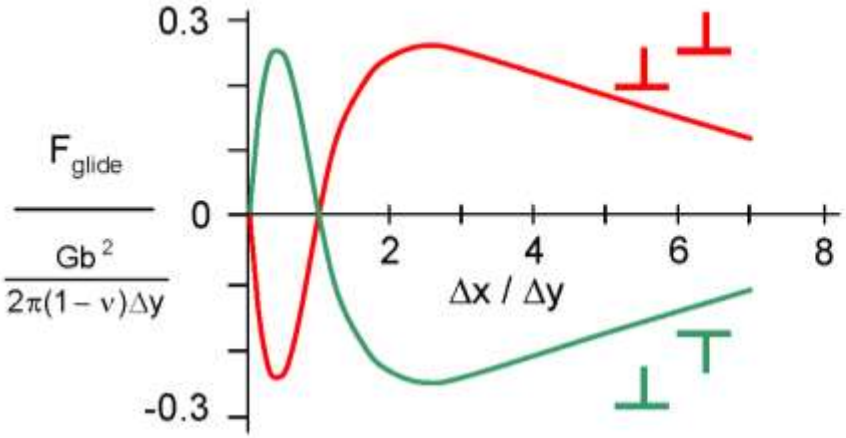
$$\sigma_{xz} = -\frac{Gb}{2\pi}\frac{\Delta y}{\Delta x^2 + \Delta y^2} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = \frac{Gb}{2\pi}\frac{\Delta x}{\Delta x^2 + \Delta y^2} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

Note that the shear stress acting to shear atoms paralle to **b** above and below the glide plane is σ_{yz}.

$$F_{res} = \sigma_{yz} b = \frac{Gb^2}{2\pi r}\cos\theta = \frac{Gb^2}{2\pi}\frac{\Delta x}{\Delta x^2 + \Delta y^2}$$

Stable configurations for dislocation ensembles



For **like** Burgers vectors:
$\Delta x = \pm\Delta y$: unstable equilibrium
$\Delta x = 0$: stable equilibrium

For **opposite** Burgers vectors:
$\Delta x = \pm\Delta y$: stable equilibrium
$\Delta x = 0$: unstable equilibrium

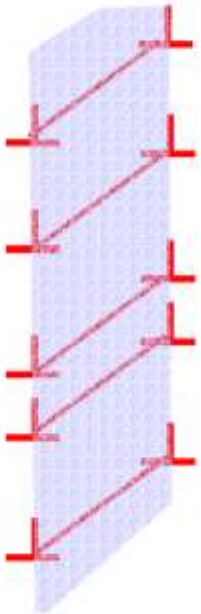
For a set of **"opposite"** Burgers vectors:

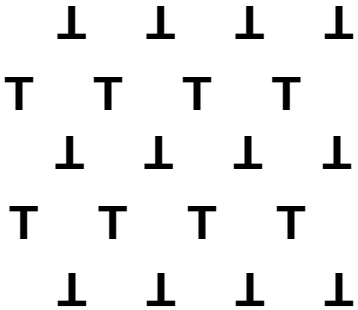
There are a large number of possible stable

For **like** Burgers vectors:
Stable array is a planar stack

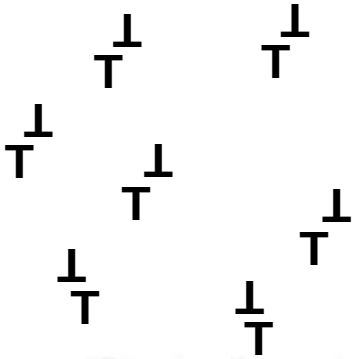
A low angle tilt boundary.

This arrangement has a strong long-range stress field.





"Taylor lattice"



"Dipole dispersion"

These stable arrangements have minimal *long-range* stress fields.

Homework: calculate forces among dislocations

Calculate the mutual forces for the following dislocation configurations:

2 parallel edge dislocations (same glide plane)
parallel edge and screw dislocations (same glide plane)
2 parallel screw dislocations (same glide plane)
2 parallel edge dislocations (above each other)
2 anti-parallel edge dislocations (same glide plane)

Write program:
store: stress fields of 2D infinite screw and edge dislocations (along z axis)
enter: position (x,y) and Burgers vector b of second dislocation (place first dislocation in origing)

Overview

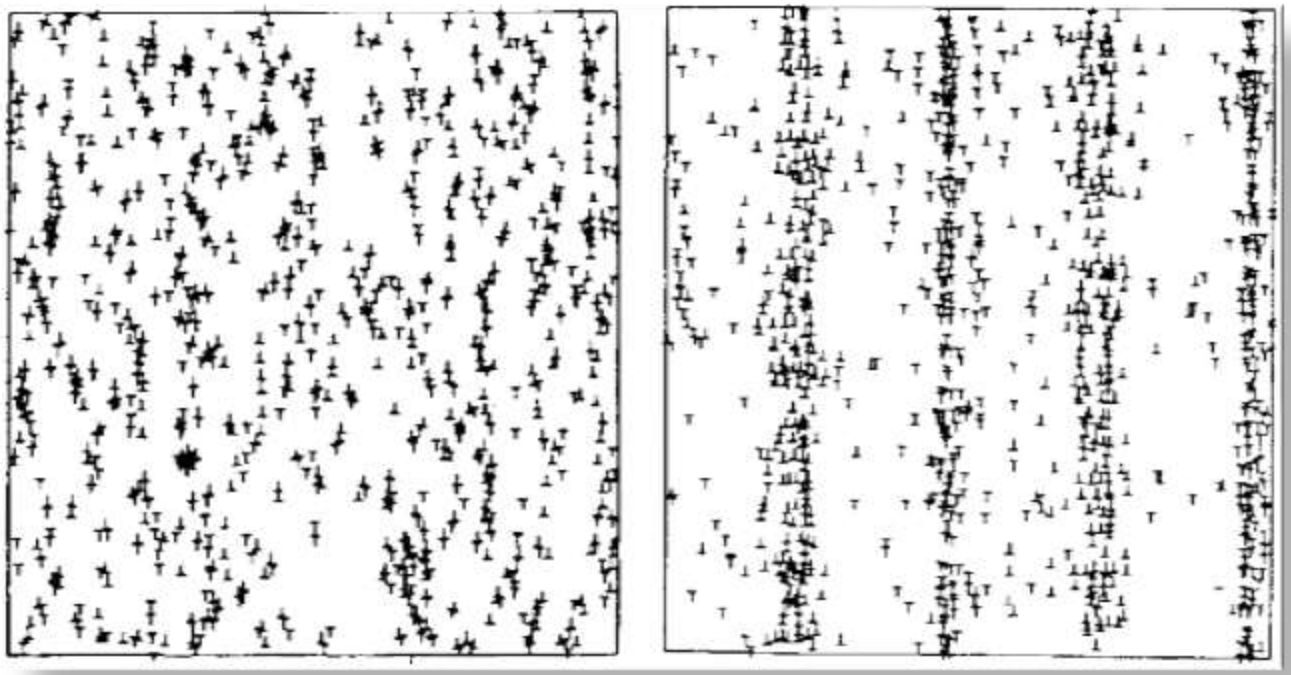
Discrete Dislocation Dynamics

Statistical Dislocation Dynamics

Discrete Dislocation Dynamics

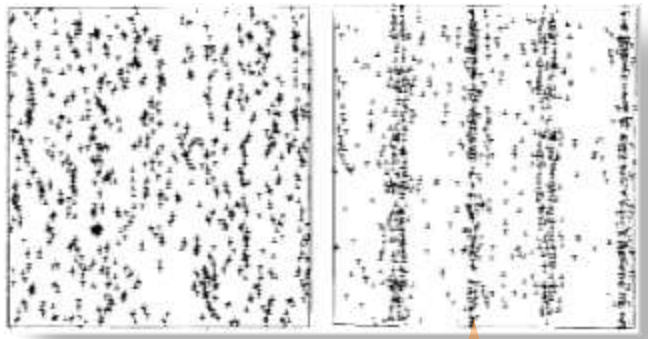
Discrete Dislocation Dynamics in 2D

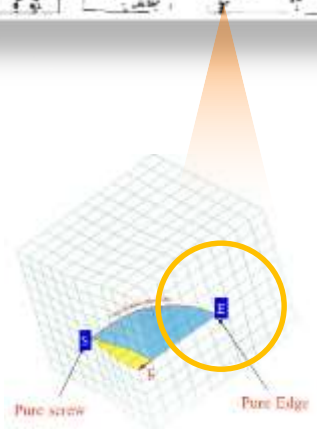
2D – view parallel to dislocation line



Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line





<u>Some questions:</u>

Difference between edge and screw dislocations?

How to do multiplication?

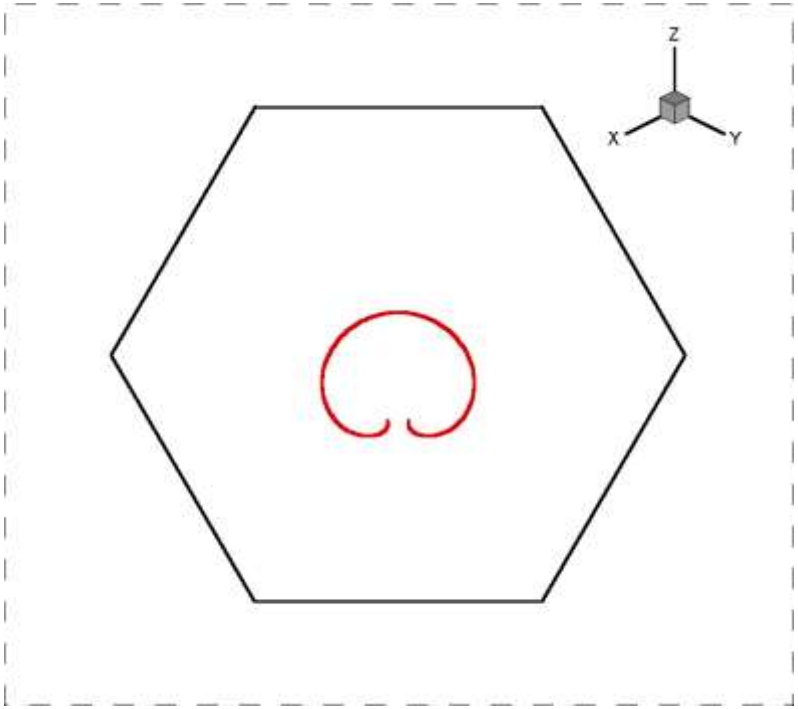
Dislocation bow-out?

Annihilation?

Climbing?

Discrete Dislocation Dynamics in 2D

2D – view into the glide plane



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

<u>Some questions:</u>

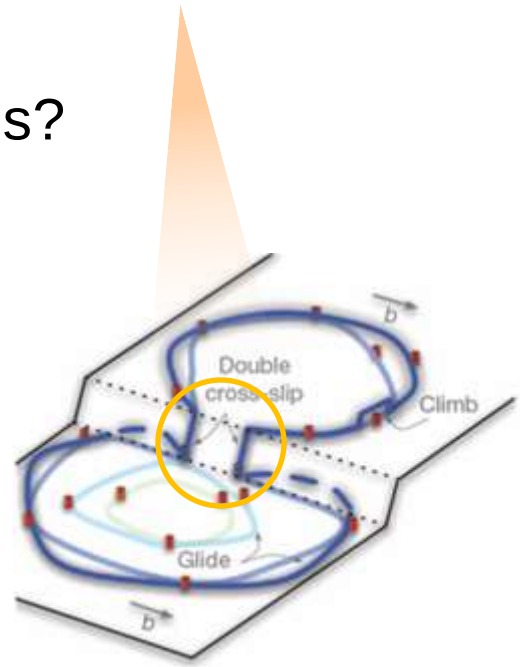
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

Jog-drag?



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

<u>Some questions:</u>

Difference between edge and screw dislocations?

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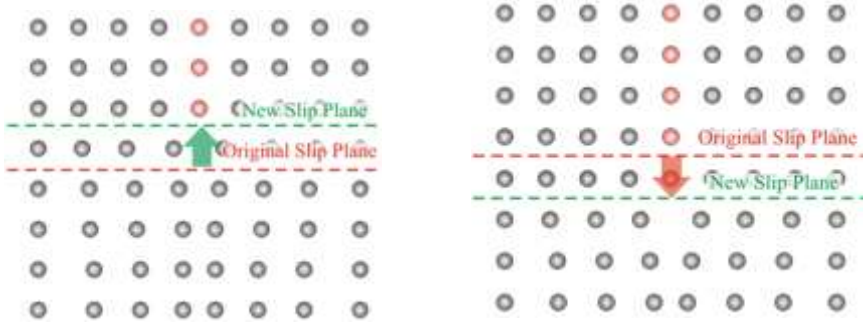


Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

<u>Some questions:</u>

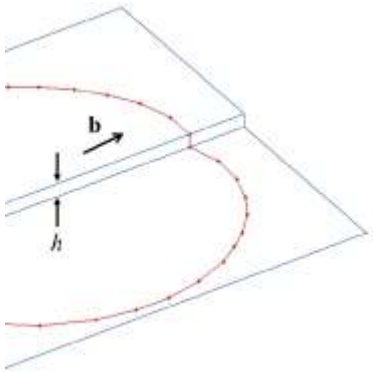
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

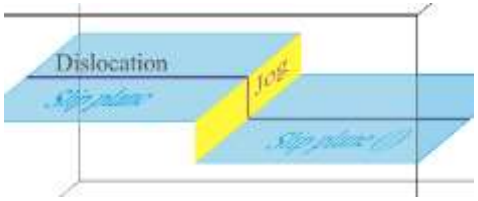
Jog-drag?



Dislocation-Dislocation Interactions

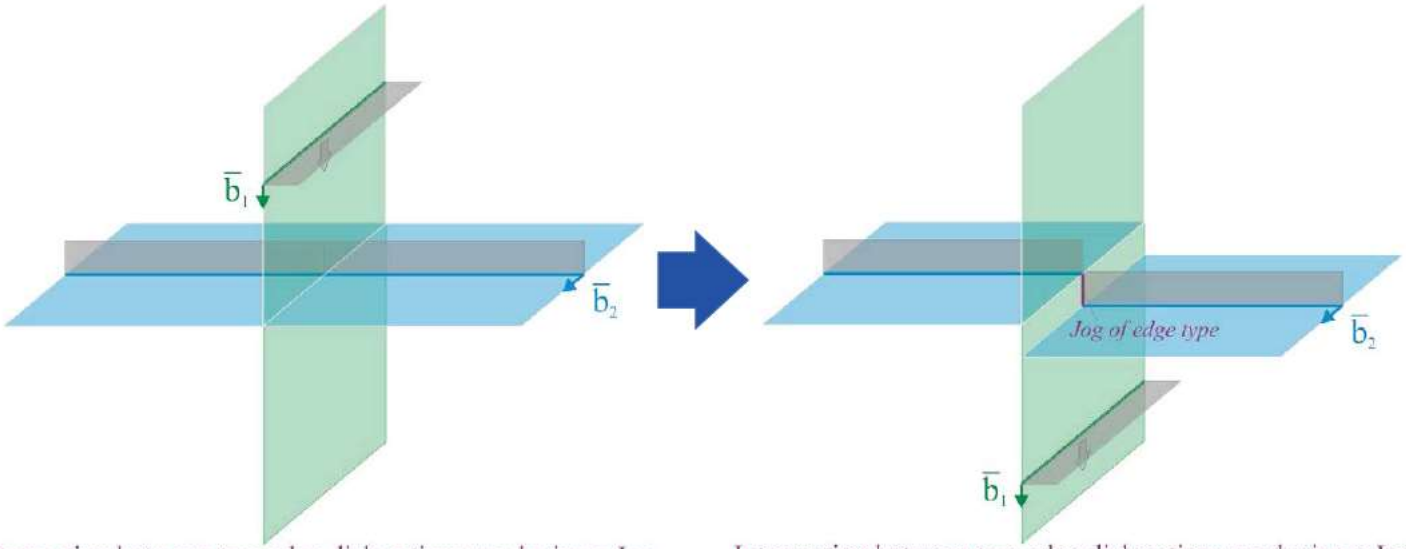
Straight dislocation can intersect to leave Jogs and Kinks in the dislocation line

Extra segments in a dislocation line cost energy and require work done by the external force



Edge-Edge Intersection Perpendicular Burgers vector

- The jog has edge character and can glide *(with Burgers vector = $\boldsymbol{b}_2$)*
- The length of the jog = $\mathbf{b}_1$.
- Edge Dislocation-1 *(Burgers vector $\mathbf{b}_1$)* is unaffected as $\mathbf{b}_2 \| \mathbf{t}_1$.
- Edge Dislocation-2 *(Burgers vector $\mathbf{b}_2$)* → Jog (Edge character) → Length $|\mathbf{b}_1|$.

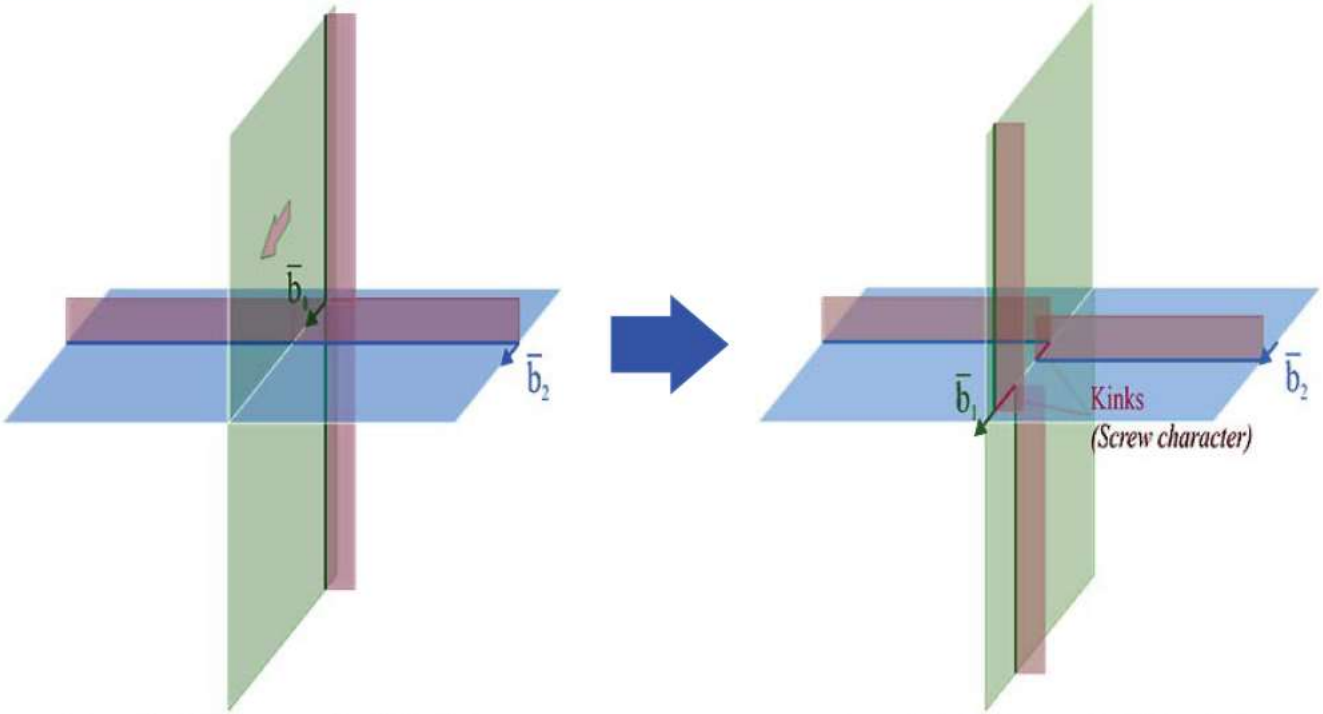


Intersection between two edge dislocations producing a Jog

Intersection between two edge dislocations producing a Jog

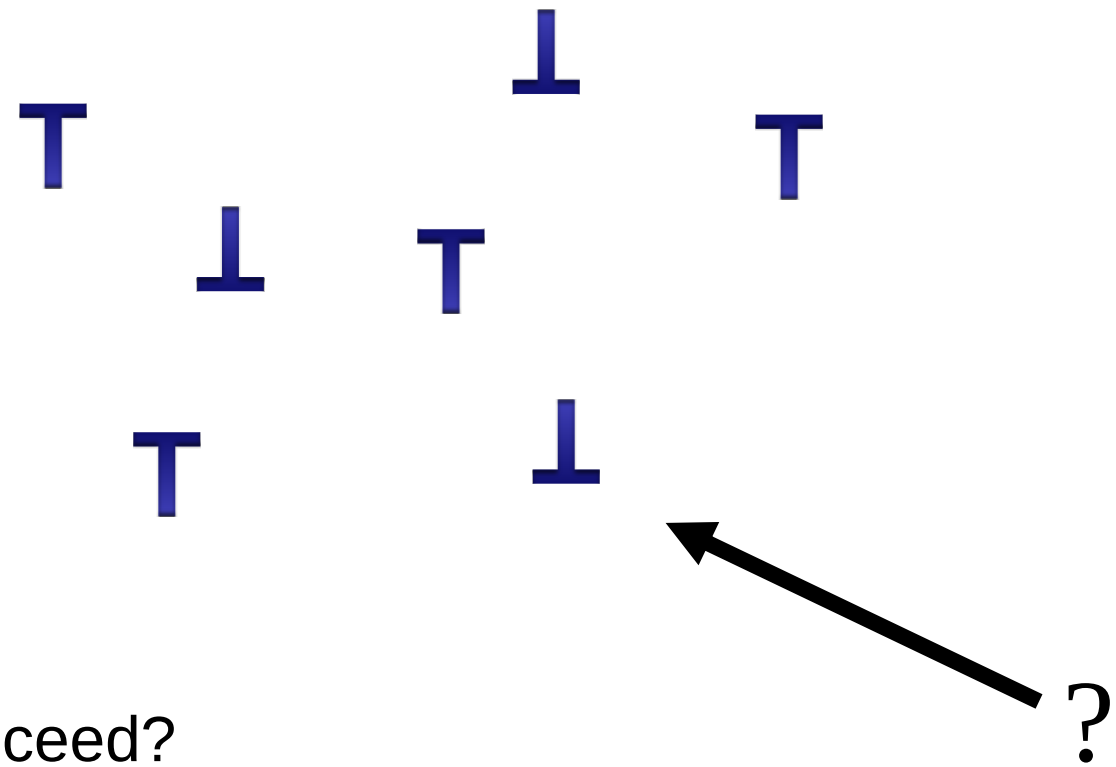
Edge-Edge Intersection Parallel Burgers vector

- Both dislocations are kinked.
- Edge Dislocation-1 *(Burgers vector* $\mathbf{b}_1$*)* → Kink (Screw character) → Length $|\mathbf{b}_2|$
- Edge Dislocation-2 *(Burgers vector* $\mathbf{b}_2$*)* → Kink (Screw character) → Length $|\mathbf{b}_1|$
- The kinks can glide



Intersection between two edge dislocations

Intersection between two edge dislocations



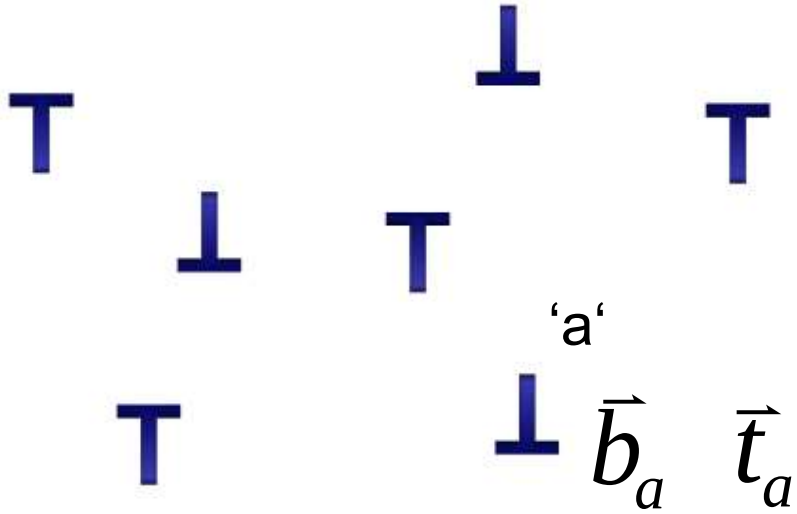
How to proceed?

Stress field of (edge) dislocation
Get coordinates
Use Peach Koehler
Move it

Force $$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{allothers} \to a} \, \vec{b}_a \right) \times \vec{t}_a$$

Force on dislocation 'a'

by all others



Force $$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{allothers}\rightarrow a} \, \vec{b}_a \right) \times \vec{t}_a$$

Motion $$\vec{F} = m \ddot{\vec{x}} + B\dot{\vec{x}} \approx B\dot{\vec{x}}$$

acceleration

friction coefficient (drag)

inertia

velocity

Equilibrium of forces

$$\sum \vec{F}_i = 0$$

$$\sum \vec{F}_i = B\dot{\vec{x}} + \vec{F}_a = 0$$

$$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{alle} \to a} \, \vec{b}_a \right) \times \vec{t}_a$$

Equilibrium of forces

$$\sum F = 0$$

$$F_{disloc} + F_{self\ force} + F_{extern} + F_{therm} + F_{viscous} + F_{obstacle} + F_{Peierls} + F_{osmotic} + F_{image} + F_{inertia}$$

F_{disloc} : elastic – other dislocations

$F_{self\ force}$: elastic – self

F_{extern} : external

F_{therm} : Stochastic Langevin

$F_{viscous}$: viscous drag

$F_{obstacle}$: obstacle

$F_{Peierls}$: Peierls

$F_{osmotic}$: chemical forces

F_{image} : surface forces

$F_{point\ defect}$: point defects

Example of Discrete Dislocation Dynamics in 2D

$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0$$

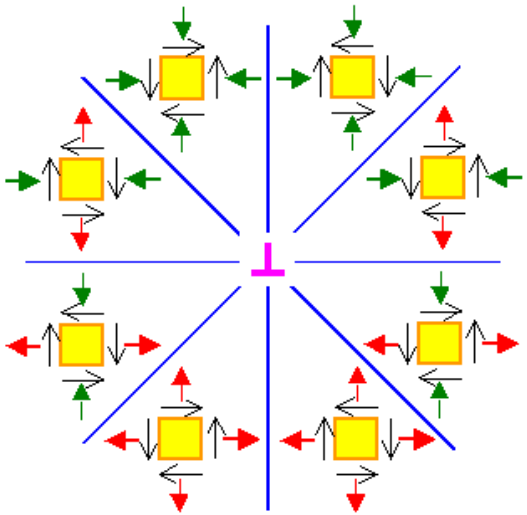
$$\sigma_{xx} = -D\,y\,\frac{3x^2 + y^2}{\left(x^2 + y^2\right)^2}, \quad \text{with:} \quad D = \frac{Gb}{2\pi(1-\nu)}$$

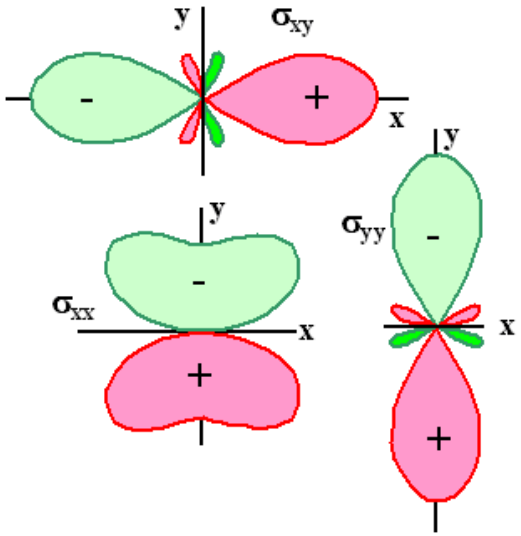
$$\sigma_{yy} = D\,y\,\frac{x^2 - y^2}{\left(x^2 + y^2\right)^2}$$

$$\sigma_{xy} = \sigma_{yx} = D\,x\,\frac{x^2 - y^2}{\left(x^2 + y^2\right)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

1





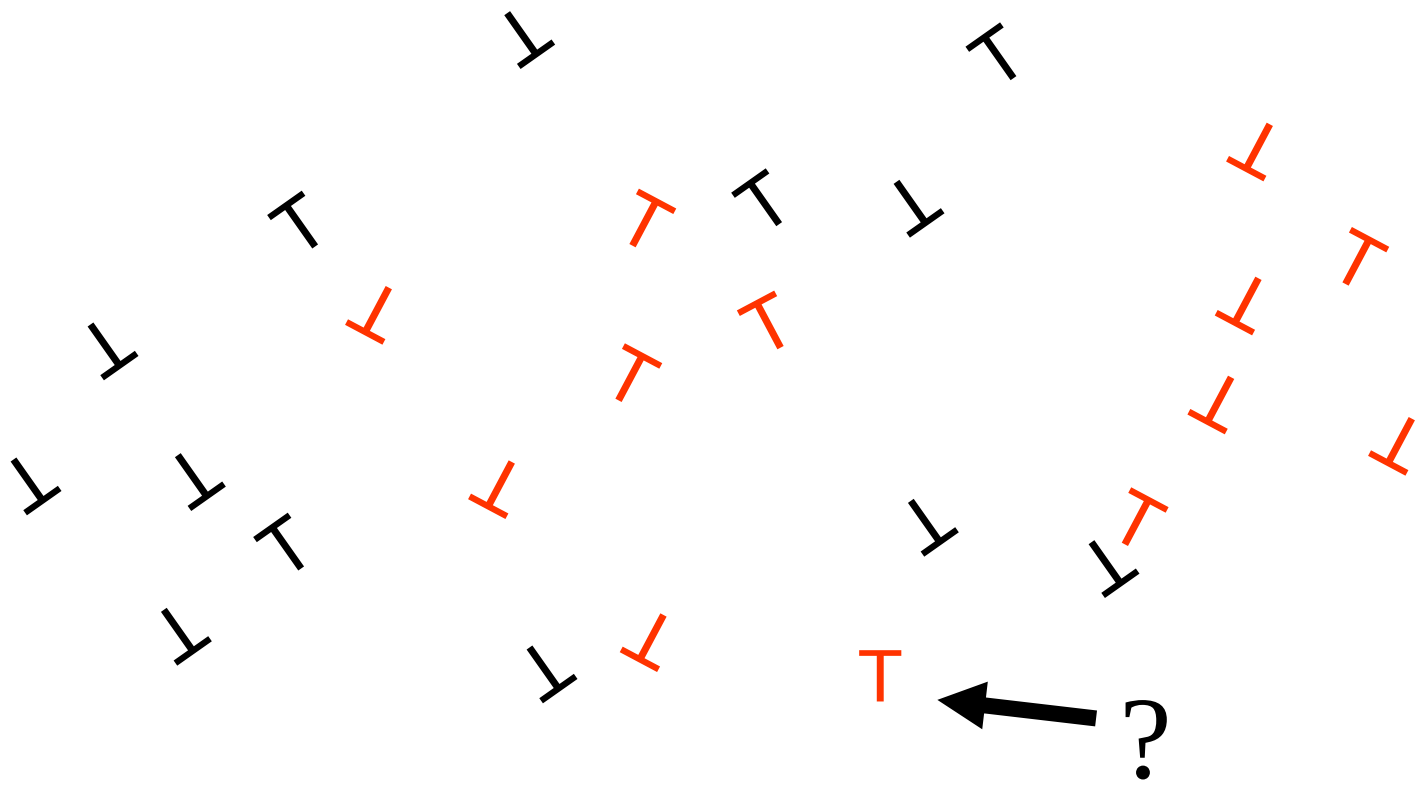
2

$$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{all}\to a}\,\vec{b}_a\right) \times \vec{t}_a$$

3

$$\vec{F}_a + B\dot{\vec{x}} + \vec{F}_{external} = 0$$

Example of Discrete Dislocation Dynamics in 2D



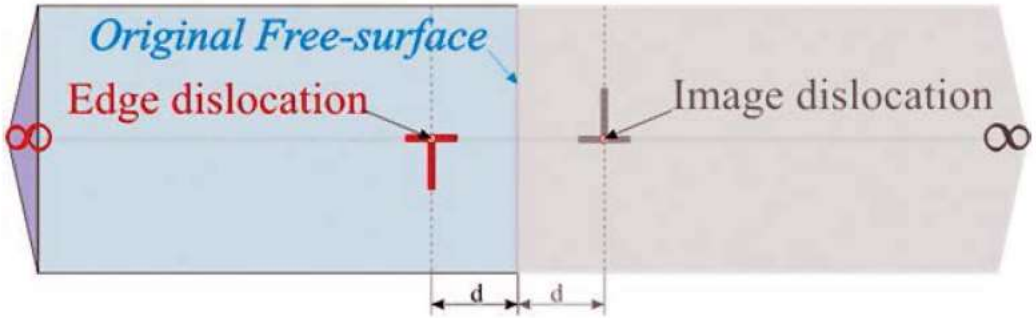
T ← ?

1) Calculate stress field of machine and of all other dislocations at position of T

2) Use Peach-Koehler equation to get force on dislocation

3) Integrate with very small time step (explicit) viscous eq. of motion

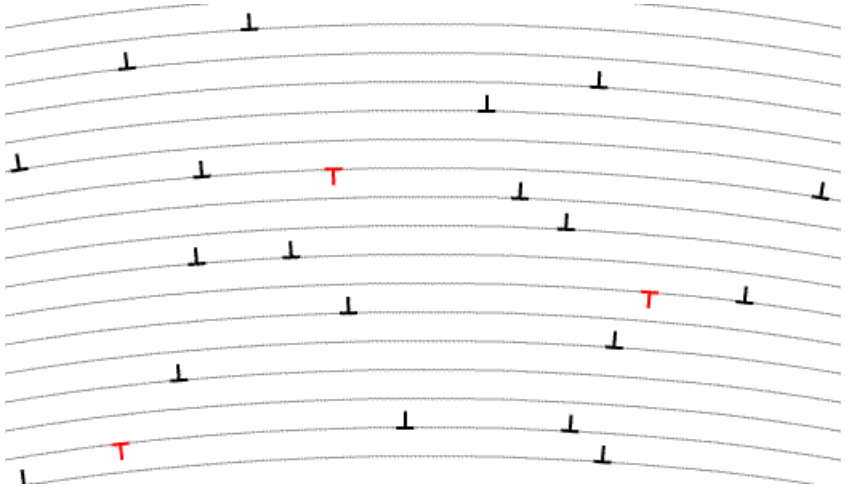
Dislocation-surface Interactions



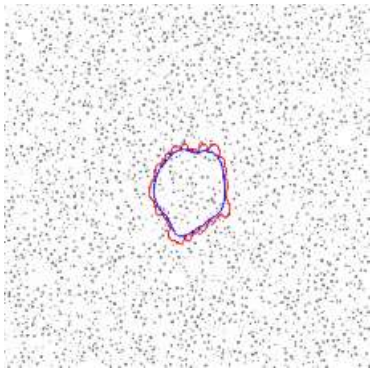
$$F_{image} = \frac{-Gb^2}{4\pi(1-\nu)d}$$

Examples

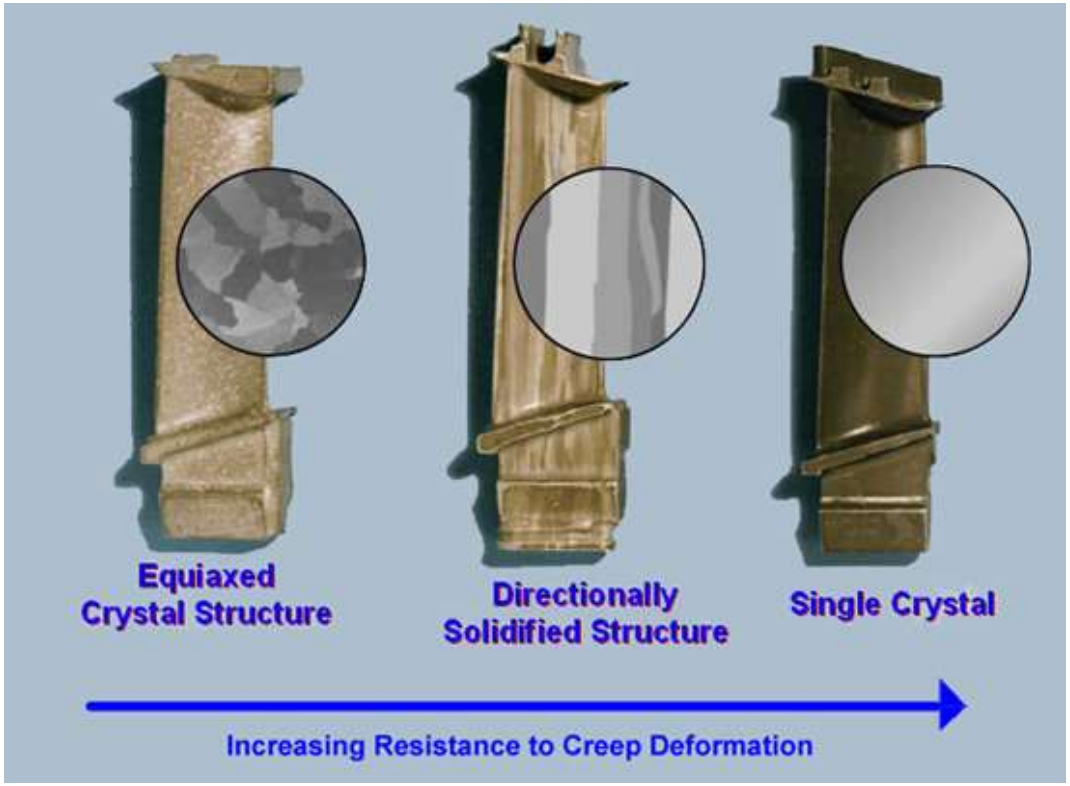
Example of Discrete Dislocation Dynamics in 2D



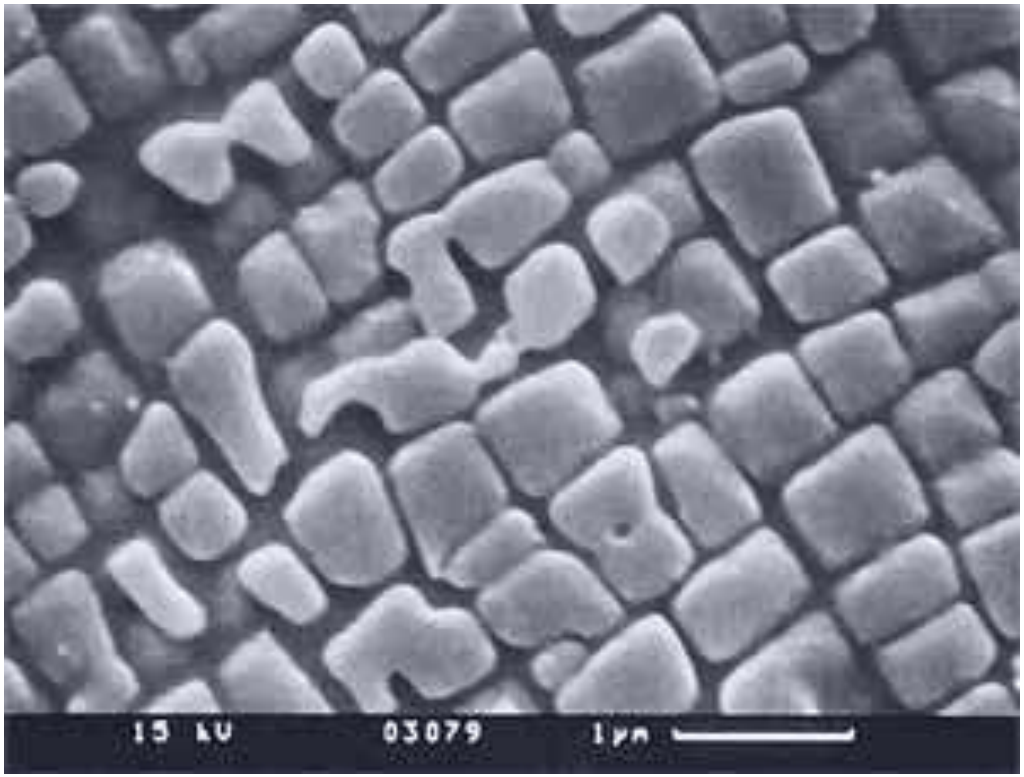
Example of Discrete Dislocation Dynamics in 2D



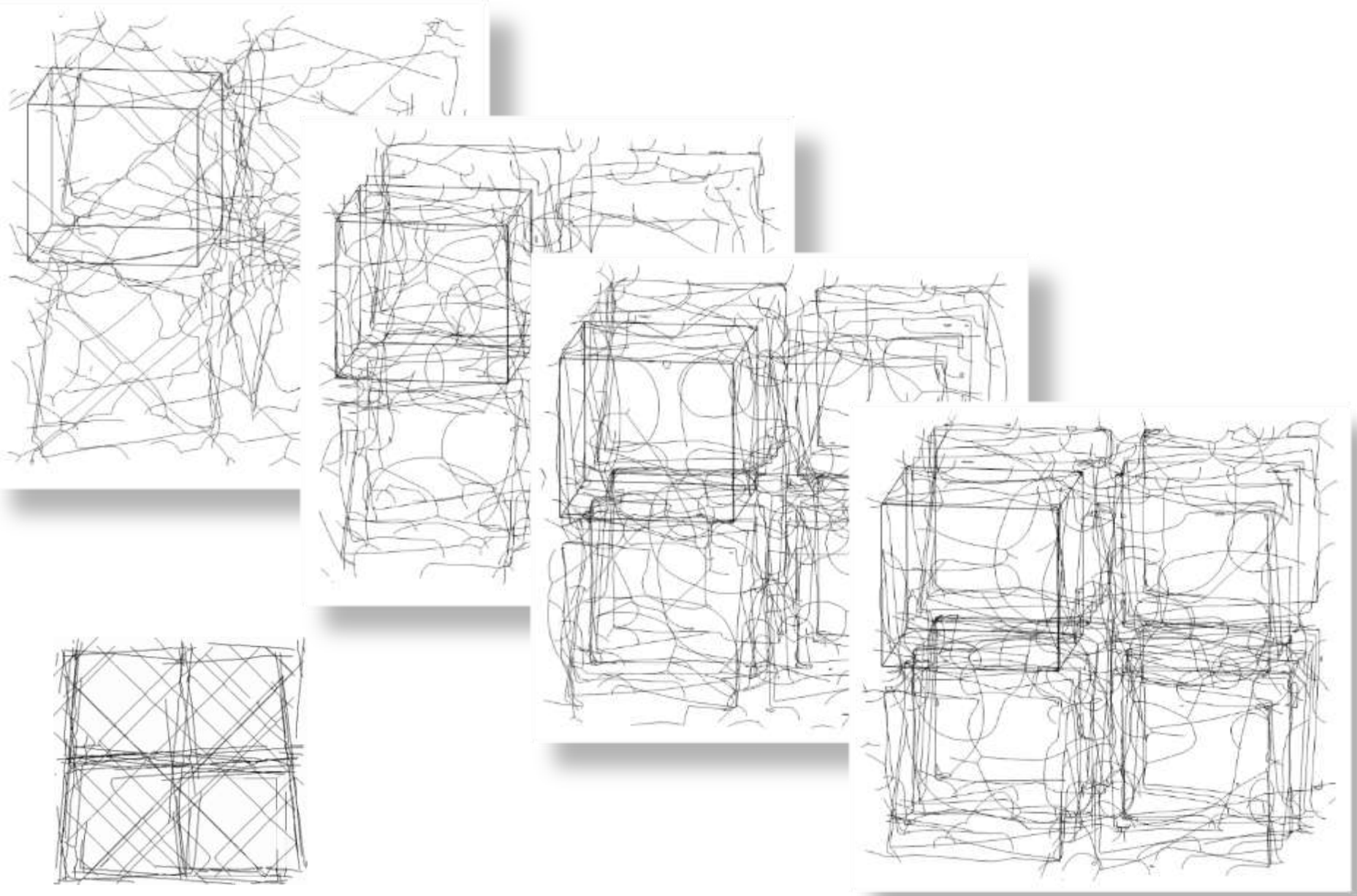
Example of Discrete Dislocation Dynamics in 3D: superalloys



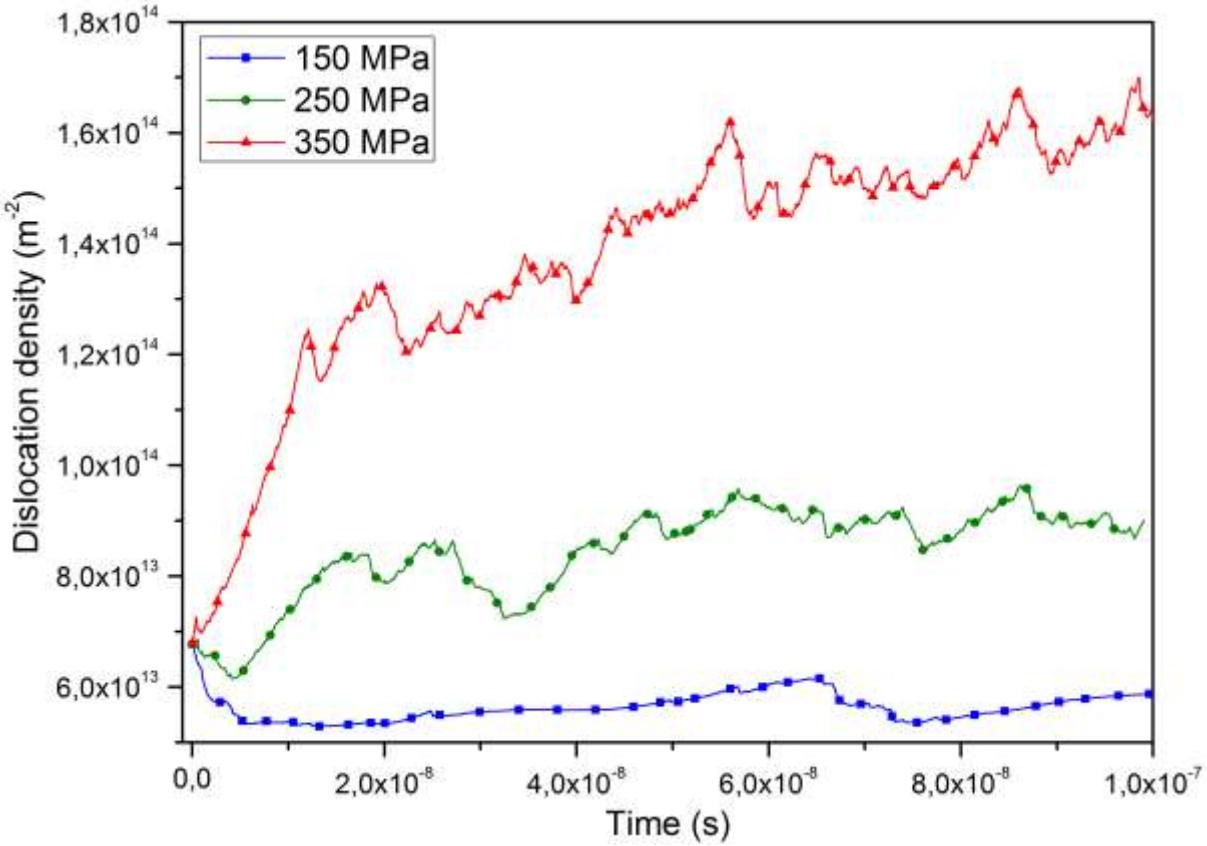
Example of Discrete Dislocation Dynamics in 3D: superalloys



Example of Discrete Dislocation Dynamics in 3D: superalloys



Example of Discrete Dislocation Dynamics in 3D: superalloys

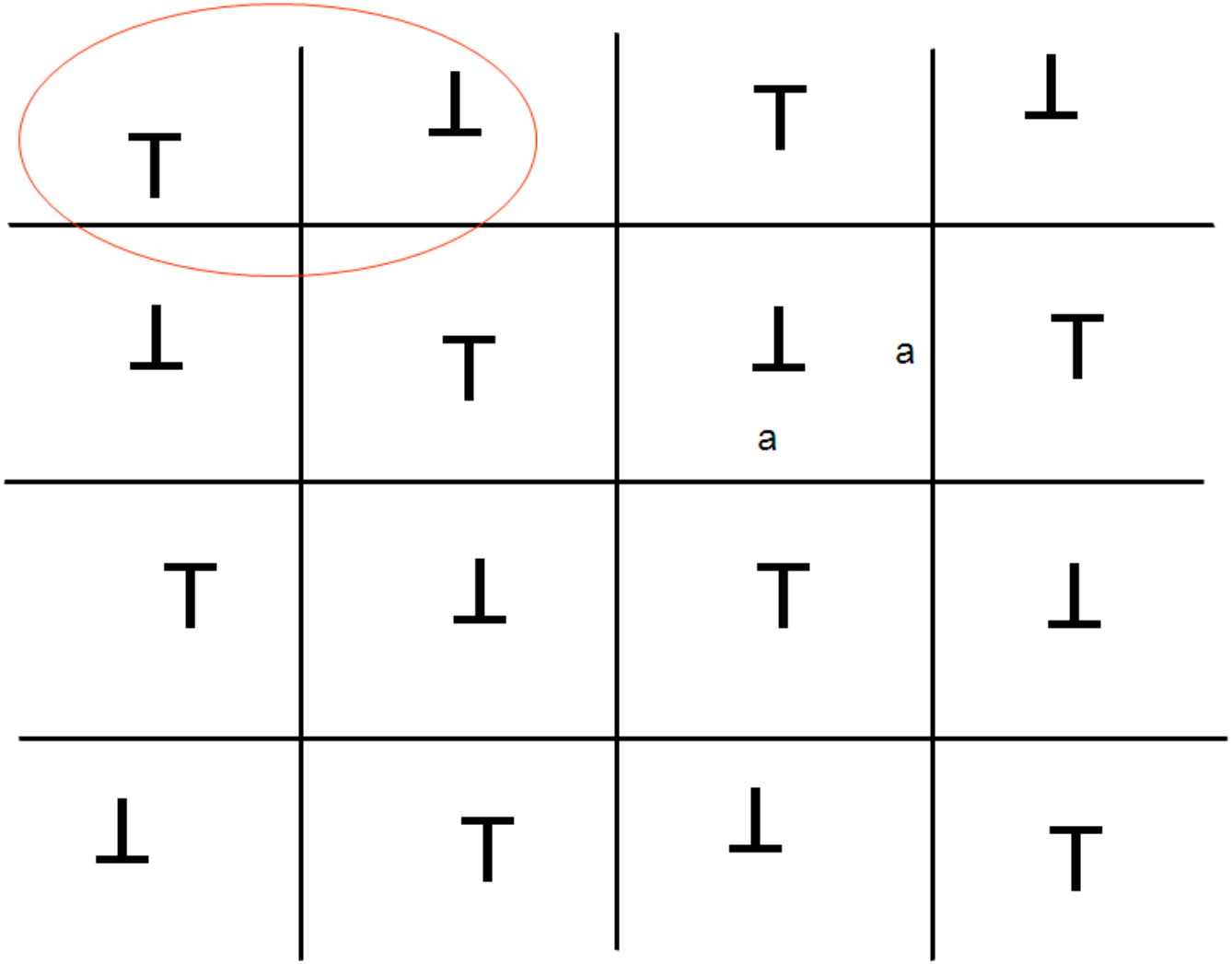


WHY Statistical Dislocation Dynamics ?

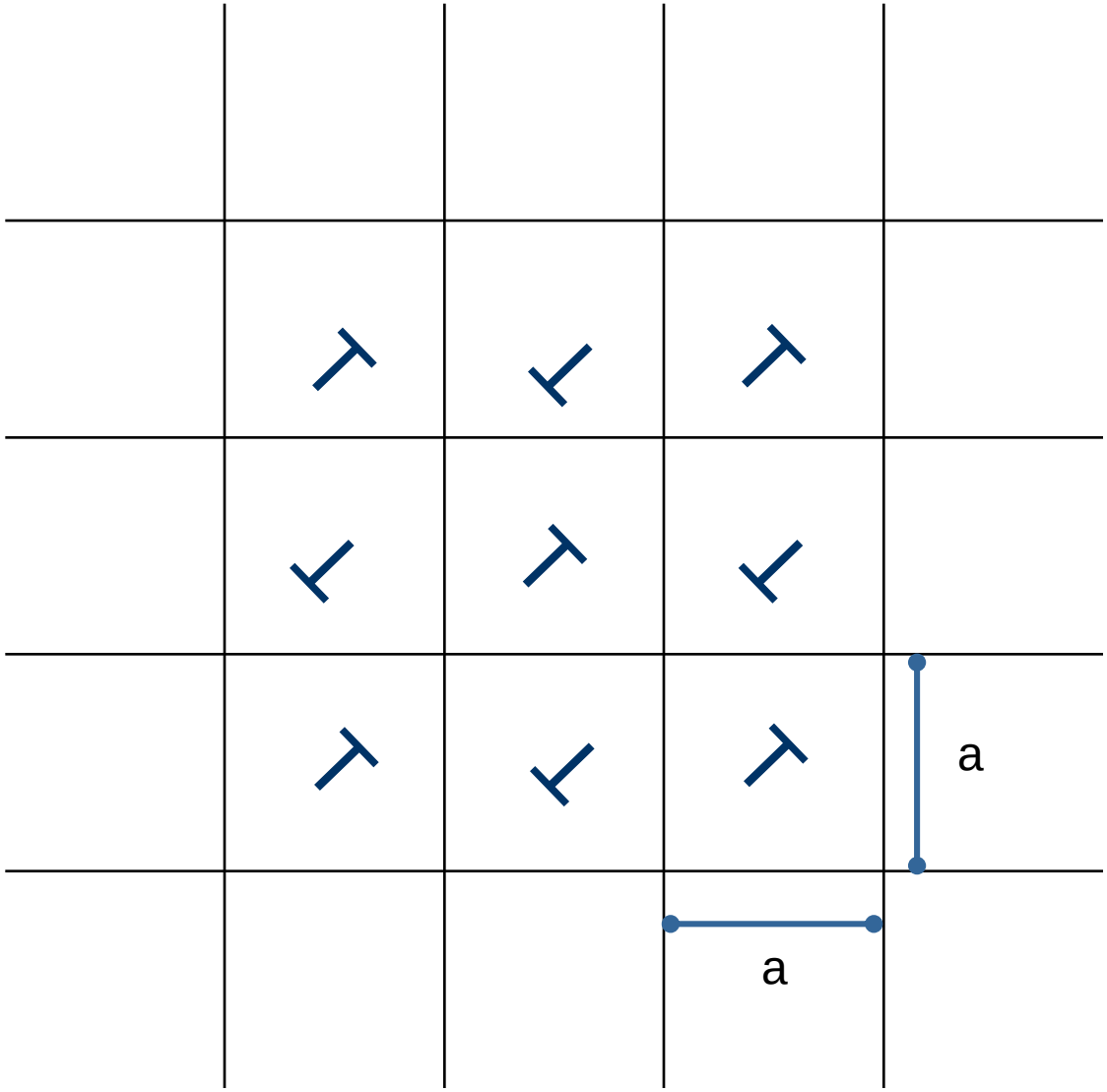
Statistical Dislocation Dynamics

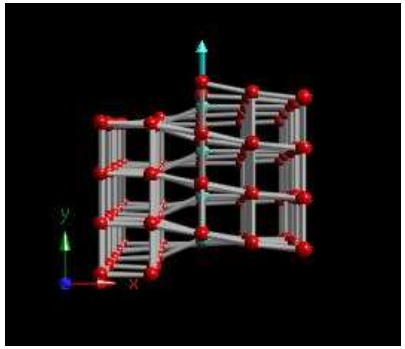
- kinetic equation of state
- structure evolution
- coupling to continuum kinematics

Statistical Dislocation Dynamics



Statistical Dislocation Dynamics



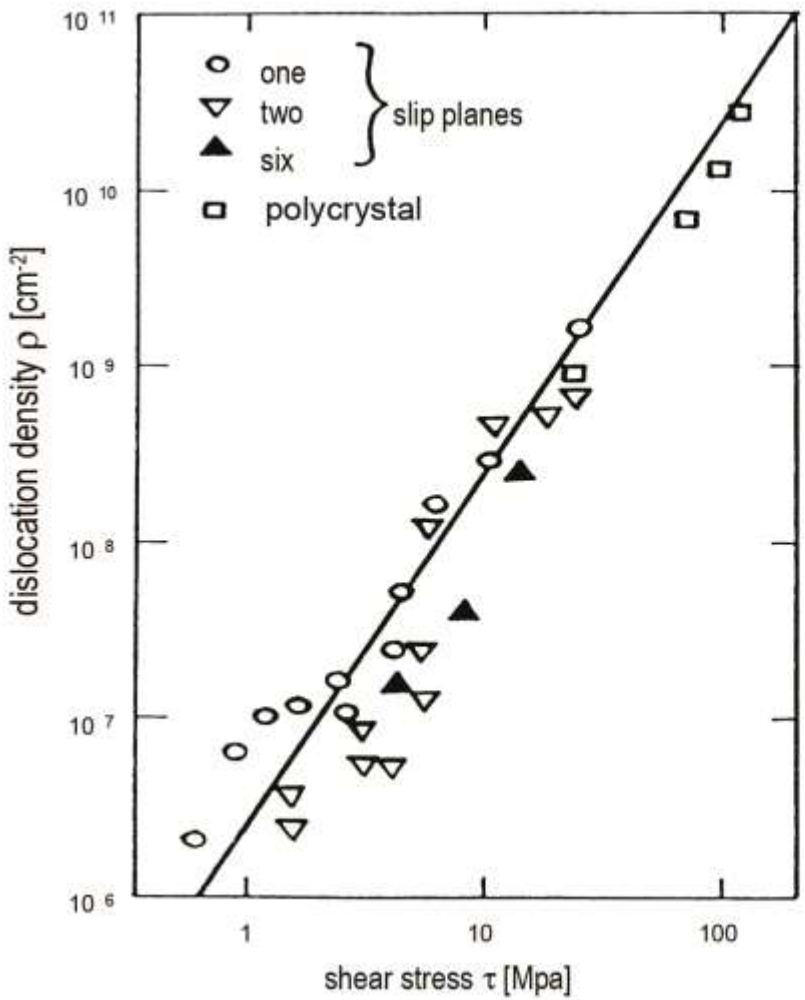


$$\tau = G\gamma = \frac{Gb}{2\pi r}$$

$$\rho = \frac{1}{a^2}$$

$$\tau = \frac{Gb}{2\pi a} = \frac{Gb}{2\pi}\sqrt{\rho}$$

- kinetic equation of state



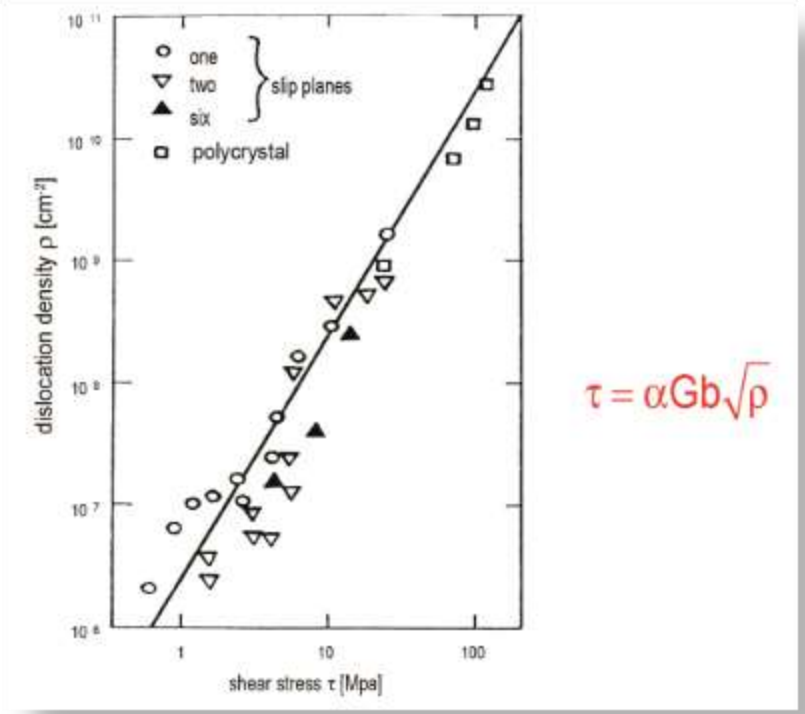
$$\tau = \alpha G b \sqrt{\rho}$$

kinetics: collective dislocation behaviour

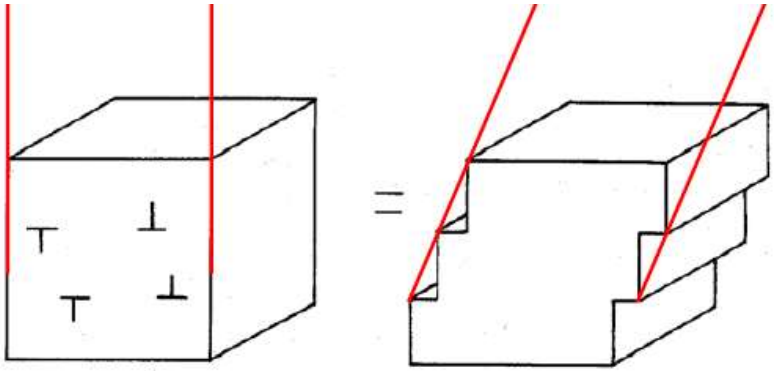
- kinetic equation of state

- structure evolution

$$\frac{d\rho}{d\gamma} = A\rho^{+} + B\rho^{-}$$



- coupling to imposed shape change



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

Microstructure Mechanics

Crystal Mechanics

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Düsseldorf, Germany
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Overview

- Single crystal yield surface
- Empirical yield surface
- Taylor model for the mechanics of polycrystals
- Examples

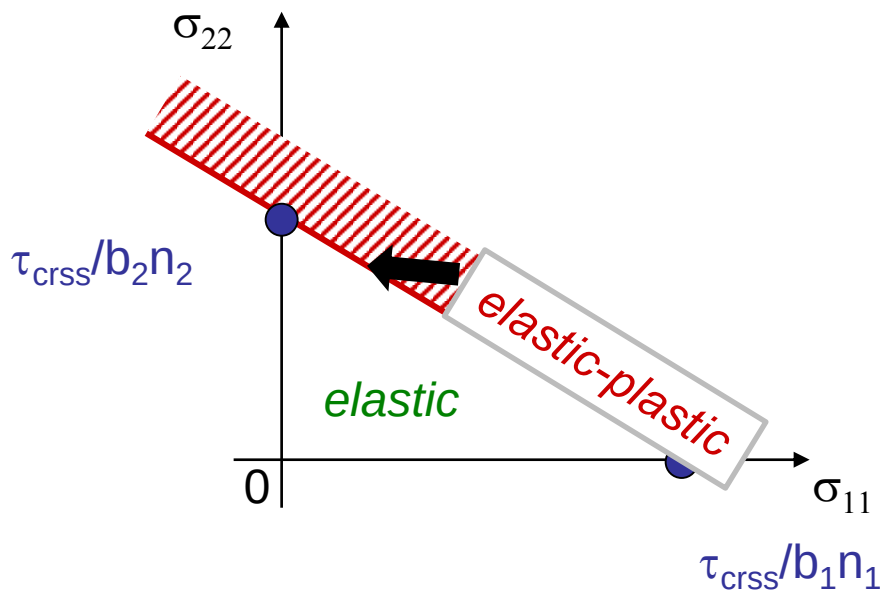
Single crystal plasticity: constructing the yield surface

- Yield criterion for single slip:

$$\sigma_{ij} b_i n_j = \tau_{crss}$$

- In 2D this becomes ($\sigma_1 \equiv \sigma_{11}$:

$$\sigma_{11} b_1 n_1 + \sigma_{22} b_2 n_2 = \tau_{crss}$$



Single crystal plasticity: constructing the yield surface

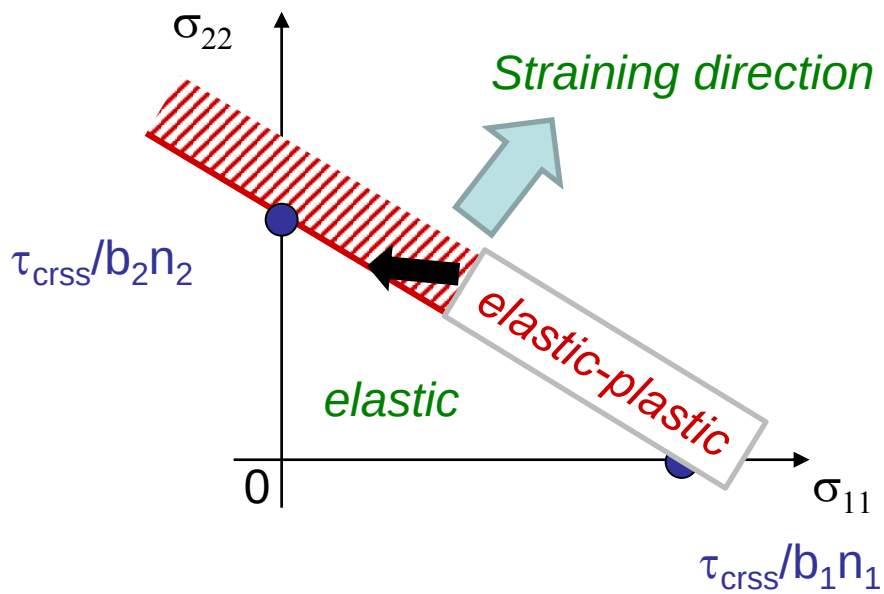
What is the straining direction?
The strain increment is given by:

$$d\varepsilon = \Sigma_s \, d\gamma^{(s)} b^{(s)} n^{(s)}$$

2D case:

$$d\varepsilon_1 = d\gamma \, b_1 n_1; \; d\varepsilon_2 = d\gamma \, b_2 n_2$$

vector perpendicular to the line for yield

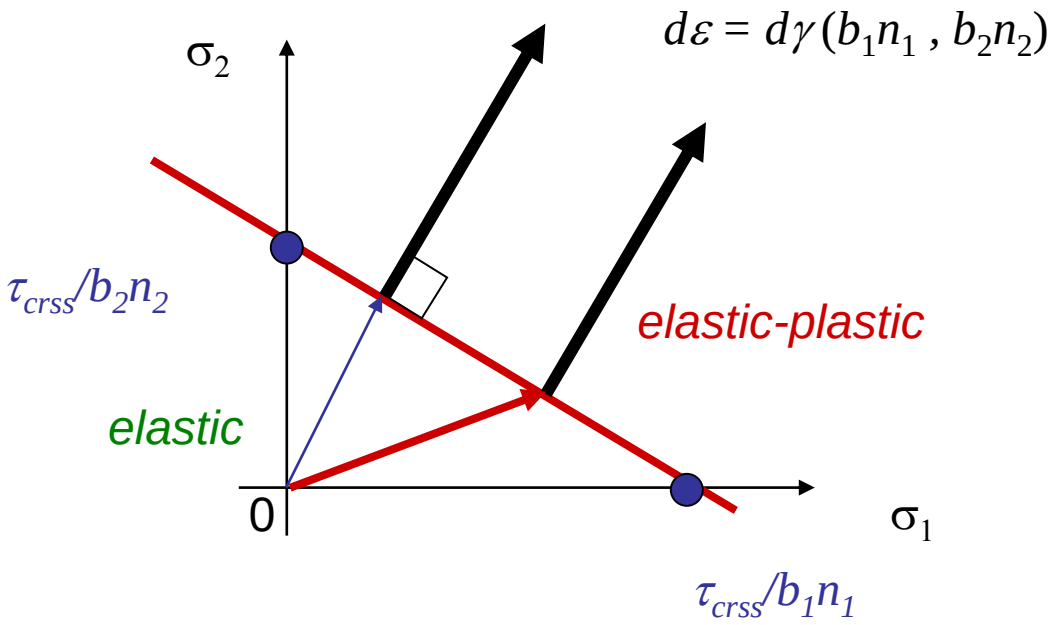


Single crystal plasticity: constructing the yield surface

straining direction in stress space

normality rule for crystallographic slip

Any given stress state can in a crystal in large-strain elasto-plasticity act only in the form of shear (except hydrostatic effects)



Active slip system:

$$\tau^{\alpha} = \tau_{\mathrm{crit}}$$

$$\tau^{\alpha} \approx \boldsymbol{T}_{\mathrm{e}} \cdot \boldsymbol{S}_0{}^{\alpha}$$

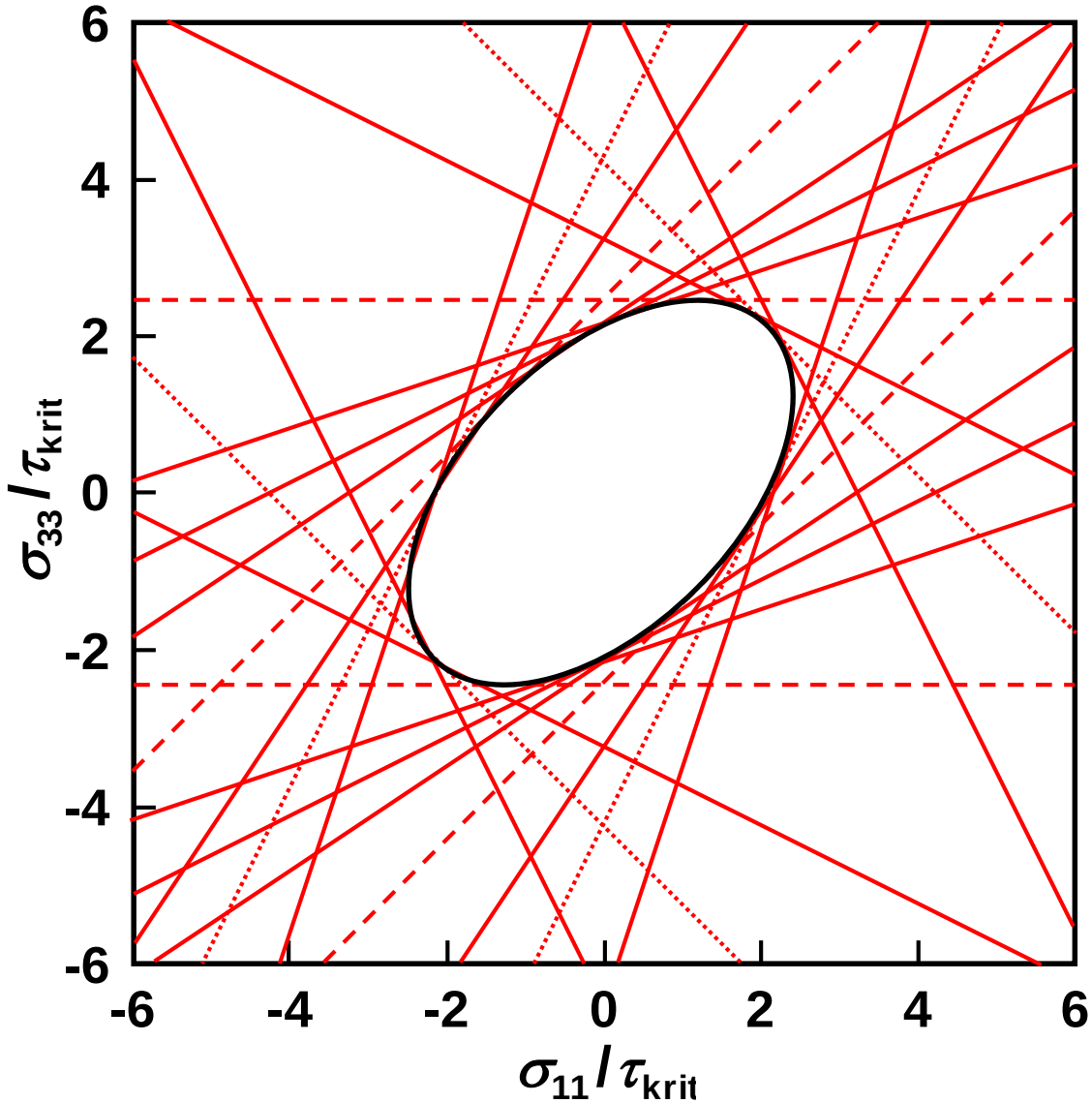
with $\boldsymbol{S}_0{}^{\alpha} = \boldsymbol{m}_0{}^{\alpha} \otimes \boldsymbol{n}_0{}^{\alpha}$

bcc 48 slip systems
orientation {001}<100>

12 x {110}<111> - - -

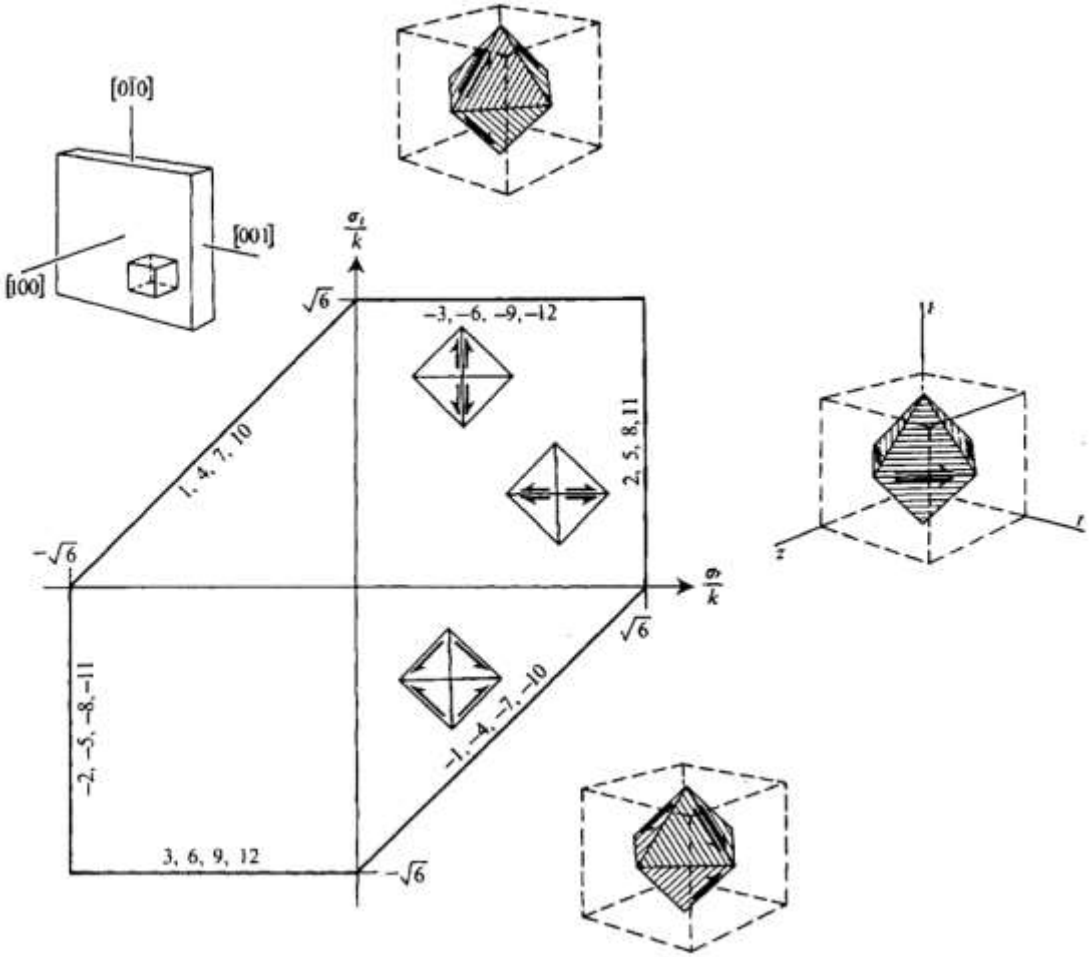
12 x {112}<111> .....

24 x {123}<111> ——



Single crystal plasticity: constructing the yield surface

Cube texture component:
(001)[100]



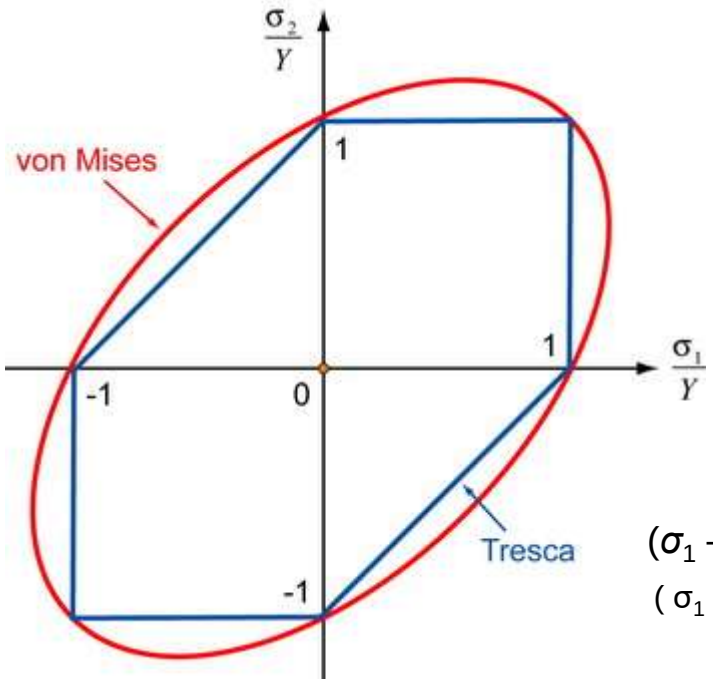
Macroscopic – empiricial yield criteria

Yield criterion: determine the critical stress required to cause permanent deformation

Many different macroscopic yield criteria

σ_{ij} stress acting on a solid
σ1, σ2, σ3 principal values of stress tensor
Y yield stress of the material in uniaxial tension

$$(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2=\text{constant}$$



$(\sigma_1 - \sigma_3) = Y$

$(\sigma_1 > \sigma_2 > \sigma_3)$

Macroscopic yield criteria

Yield criterion: determine the critical stress required to cause permanent deformation

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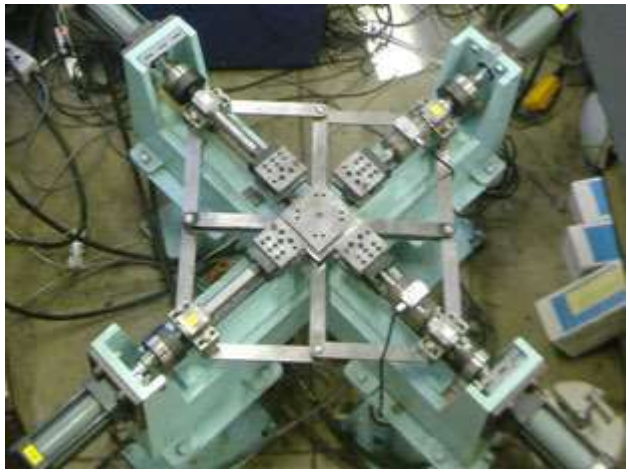
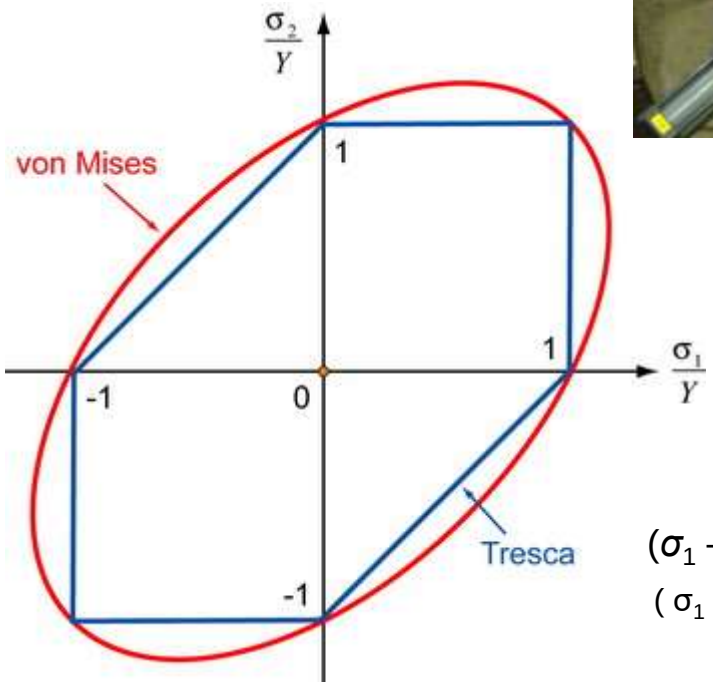
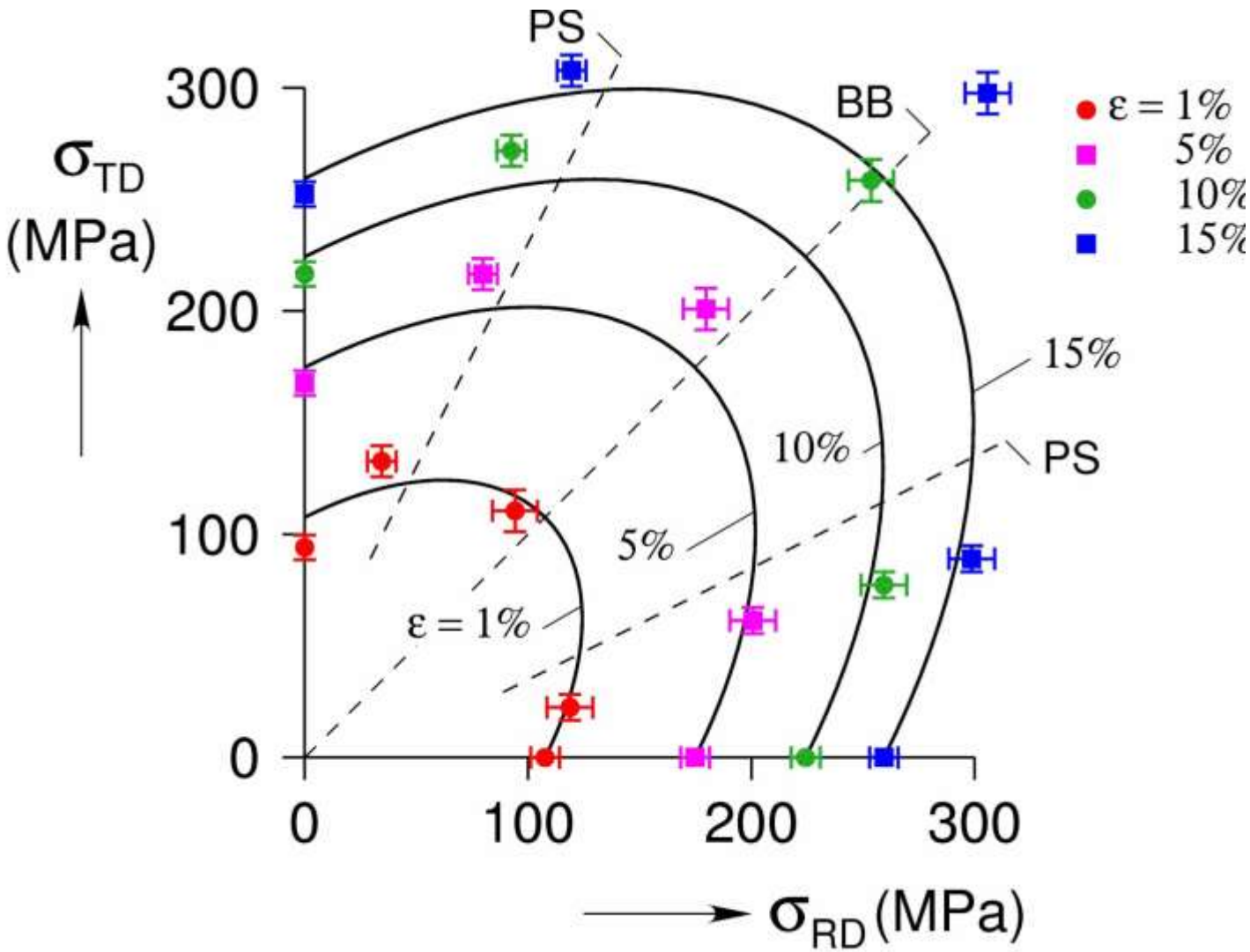


$$(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2=\text{constant}$$



$(\sigma_1 - \sigma_3) = Y$

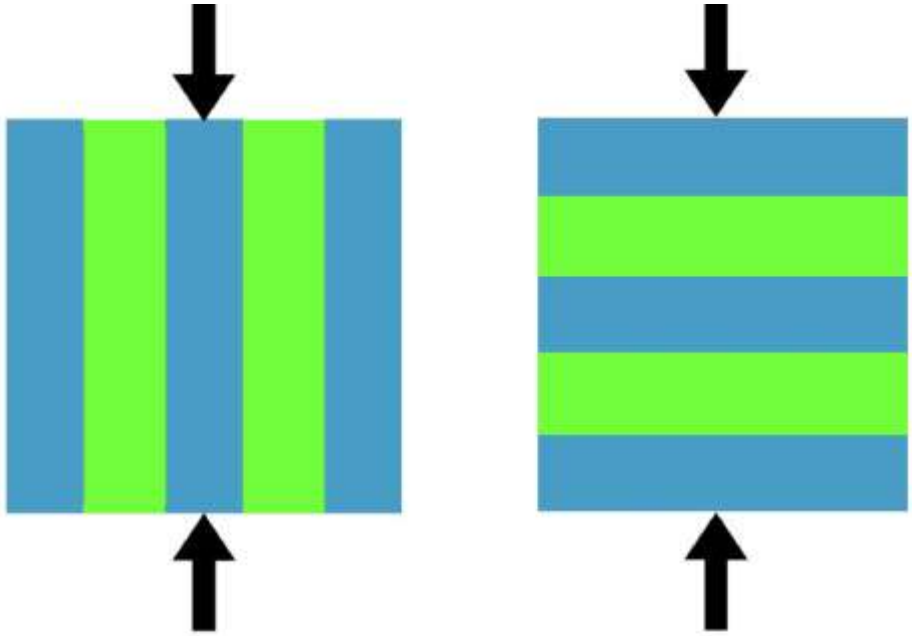
$(\sigma_1 > \sigma_2 > \sigma_3)$


PS
BB
300
200
100
0
σ_{TD}
(MPa)
ε = 1%
5%
10%
15%
15%
10%
PS
5%
ε = 1%
0
100
200
300
σ_{RD} (MPa)

Overview

- How does that work for bicrystals ?
- Two extreme cases :
- iso-strain (Taylor)
- iso-stress (Schmid)

Iso-stress and iso-strain: general approach



Isostrain	Isostress
$\varepsilon = \varepsilon_s = \varepsilon_d$	$\varepsilon = \varepsilon_s + \varepsilon_d$
$\sigma = \sigma_s + \sigma_d$	$\sigma = \sigma_s = \sigma_d$
Displacement continuity across layers	Stress continuity across layers

Iso-stress and iso-strain: Elastic approach: composite stiffness

Bounding Case - Isostrain

$$\epsilon_1 = \epsilon_2 = \epsilon_{tot}$$

$$\sigma_1 = E_1\epsilon_1 = E_1\epsilon_{tot} \quad ; \quad \sigma_2 = E_2\epsilon_2 = E_2\epsilon_{tot}$$

$$P_1 = A_1\sigma_1 = A_1E_1\epsilon_{tot} \quad ; \quad P_2 = A_2\sigma_2 = A_2E_2\epsilon_{tot}$$

$$P_{tot} = P_1 + P_2 = \epsilon_{tot}(A_1E_1 + A_2E_2)$$

$$\sigma_{tot} = \frac{P_{tot}}{A_1 + A_2} = \epsilon_{tot}\left(\frac{A_1}{A_1 + A_2}E_1 + \frac{A_2}{A_1 + A_2}E_2\right)$$

$$\sigma_{tot} = (f_1E_1 + f_2E_2)\epsilon_{tot}$$

$$\boxed{E_{tot} = f_1E_1 + f_2E_2}$$

P_1, P_2 are the loads on 1 and 2.

f_1, f_2 are the volume fractions of 1 and 2.

Bounding Case - Isostress

$$\sigma_1 = \sigma_2 = \sigma_{tot}$$

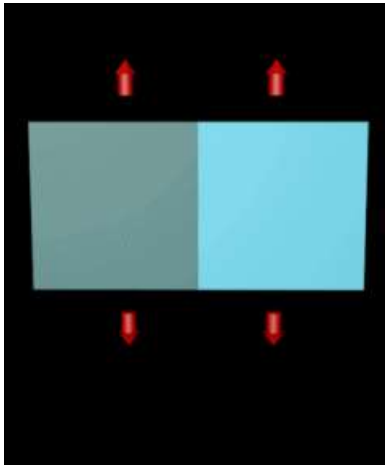
$$\sigma_1 = E_1\epsilon_1 \quad ; \quad \sigma_2 = E_2\epsilon_2$$

$$\epsilon_{tot} = f_1\epsilon_1 + f_2\epsilon_2 = f_1\frac{\sigma_{tot}}{E_1} + f_2\frac{\sigma_{tot}}{E_2}$$

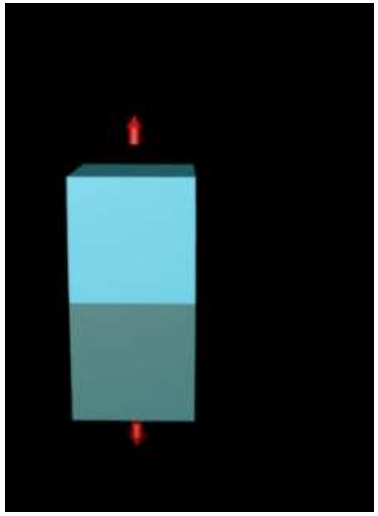
$$\boxed{E = \frac{\sigma_{tot}}{\epsilon_{tot}} = \frac{1}{\frac{f_1}{\epsilon_1} + \frac{f_2}{\epsilon_2}} = \frac{E_1E_2}{f_1E_2 + f_2E_1}}$$

Iso-stress and iso-strain

- iso-strain (Taylor-model)



- iso-stress (Sachs-model)



Roters et al. Acta Mater. 58 (2010)

Iso-stress and iso-strain for polycrystals

Sachs Model (previous lecture on single crystal):

- All grains with aggregate or polycrystal experience the same state of stress;
- Equilibrium condition across the grain boundaries satisfied;
- Compatibility conditions between the grains violated, thus, finite strains will lead to gaps and overlaps between grains;
- Generally most successful for single crystal deformation with *stress boundary conditions on each grain*.

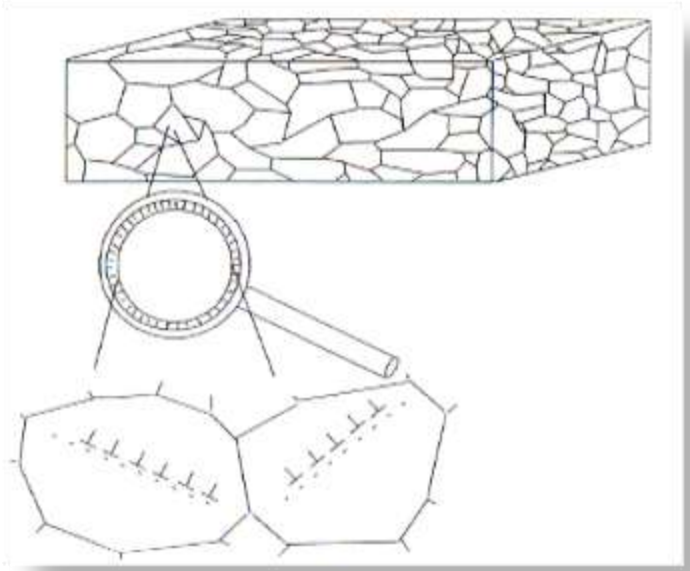
Taylor Model (this lecture):

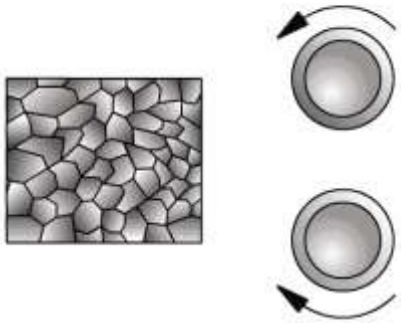
- All single-crystal grains within the aggregate experience the same state of deformation (strain);
- Equilibrium condition across the grain boundaries violated, because the vertex stress states required to activate multiple slip in each grain vary from grain to grain;
- Compatibility conditions between the grains satisfied;
- Generally most successful for polycrystals with strain boundary conditions on each grain.

Polycrystal model

- Taylor model for the mechanics of polycrystals

The Taylor Model



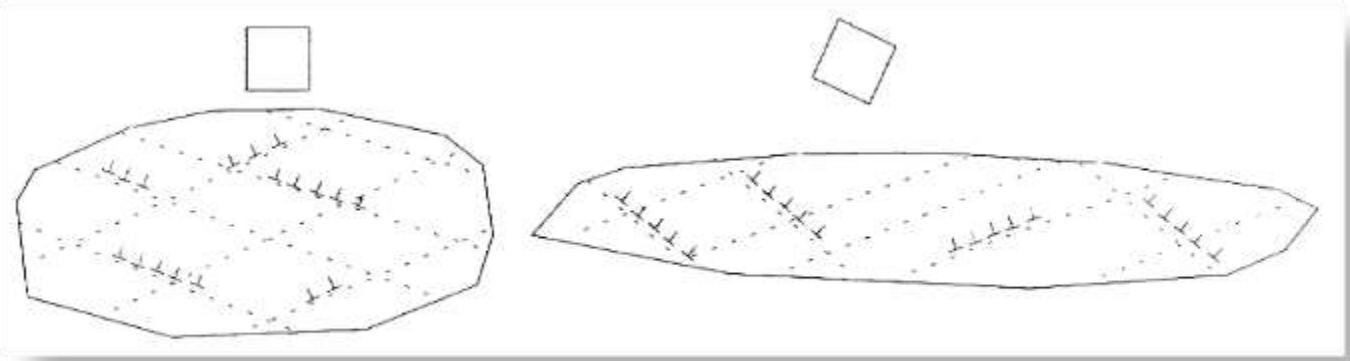


Cold Rolling

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

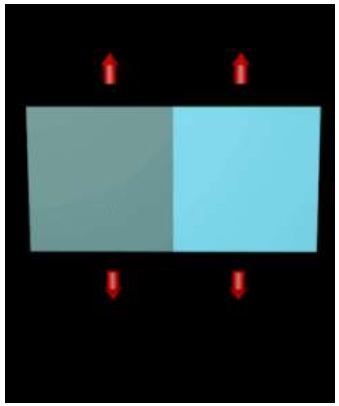
The Taylor Model

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



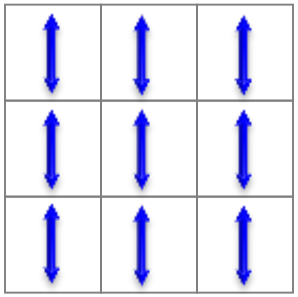
plastic spin from polar decomposition

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



The Taylor Model – comparison to Sachs model

External Stress

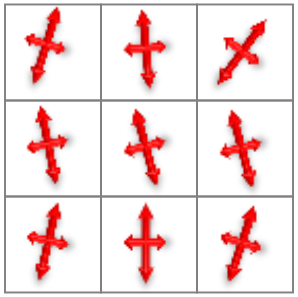


Increasing strain

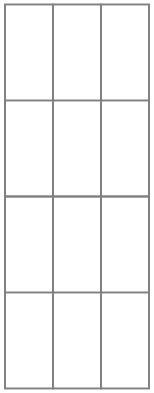
Small arrows indicate identical stress state in each grain

Each grain deforms according to which single slip system is active

External Strain



Small arrows indicate variable stress state in each grain



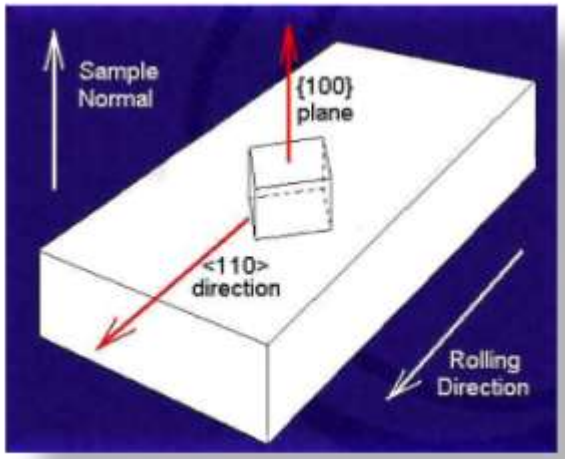
Multiple slip (with 5 or more systems) in each grain satisfies the externally imposed strain, *D*

The Taylor Model – comparison to Sachs model

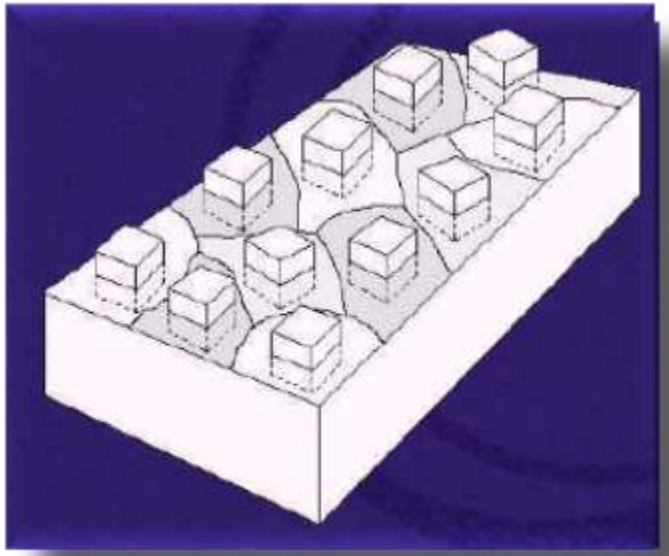
$$\begin{bmatrix} D_2 \\ D_3 \\ D_4 \\ D_5 \\ D_6 \end{bmatrix} = \begin{bmatrix} m_{22}^{(1)} & m_{22}^{(2)} & m_{22}^{(3)} & m_{22}^{(4)} & m_{22}^{(5)} \\ m_{33}^{(1)} & m_{33}^{(2)} & m_{33}^{(3)} & m_{33}^{(4)} & m_{33}^{(5)} \\ (m_{23}^{(1)}+m_{32}^{(1)}) & (m_{23}^{(2)}+m_{32}^{(2)}) & (m_{23}^{(3)}+m_{32}^{(3)}) & (m_{23}^{(4)}+m_{32}^{(4)}) & (m_{23}^{(5)}+m_{32}^{(5)}) \\ (m_{13}^{(1)}+m_{31}^{(1)}) & (m_{13}^{(2)}+m_{31}^{(2)}) & (m_{13}^{(3)}+m_{31}^{(3)}) & (m_{13}^{(4)}+m_{31}^{(4)}) & (m_{13}^{(5)}+m_{31}^{(5)}) \\ (m_{12}^{(1)}+m_{21}^{(1)}) & (m_{12}^{(2)}+m_{21}^{(2)}) & (m_{12}^{(3)}+m_{21}^{(3)}) & (m_{12}^{(4)}+m_{21}^{(4)}) & (m_{12}^{(5)}+m_{21}^{(5)}) \end{bmatrix} \begin{bmatrix} d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \\ d\gamma_4 \\ d\gamma_5 \end{bmatrix}$$

$$\begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \\ \tau_5 \end{bmatrix} = \begin{bmatrix} m_{11}^{(1)} m_{22}^{(1)} m_{33}^{(1)} & (m_{23}^{(1)}+m_{32}^{(1)}) & (m_{13}^{(1)}+m_{31}^{(1)}) & (m_{12}^{(1)}+m_{21}^{(1)}) \\ m_{11}^{(2)} m_{22}^{(2)} m_{33}^{(2)} & (m_{23}^{(2)}+m_{32}^{(2)}) & (m_{13}^{(2)}+m_{31}^{(2)}) & (m_{12}^{(2)}+m_{21}^{(2)}) \\ m_{11}^{(3)} m_{22}^{(3)} m_{33}^{(3)} & (m_{23}^{(3)}+m_{32}^{(3)}) & (m_{13}^{(3)}+m_{31}^{(3)}) & (m_{12}^{(3)}+m_{21}^{(3)}) \\ m_{11}^{(4)} m_{22}^{(4)} m_{33}^{(4)} & (m_{23}^{(4)}+m_{32}^{(4)}) & (m_{13}^{(4)}+m_{31}^{(4)}) & (m_{12}^{(4)}+m_{21}^{(4)}) \\ m_{11}^{(5)} m_{22}^{(5)} m_{33}^{(5)} & (m_{23}^{(5)}+m_{32}^{(5)}) & (m_{13}^{(5)}+m_{31}^{(5)}) & (m_{12}^{(5)}+m_{21}^{(5)}) \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}$$

Crystal rotations under heterogeneous constraints



Grains in polycrystals do NOT experience the same boundary conditions.



Differentiate between GLOBAL bounday conditions (tool, process) and the LOCAL (micromechanical) boundary conditions. The latter are influenced by grain-to-grain interactions and local inhomogeneity.

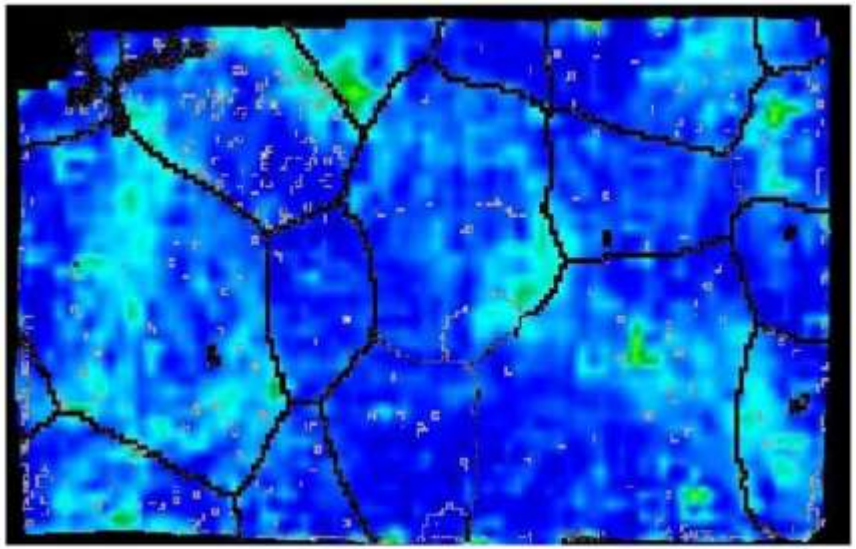
Raabe et al. Acta Mat. 49 (2001)

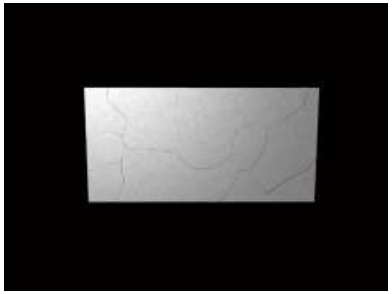
Overview

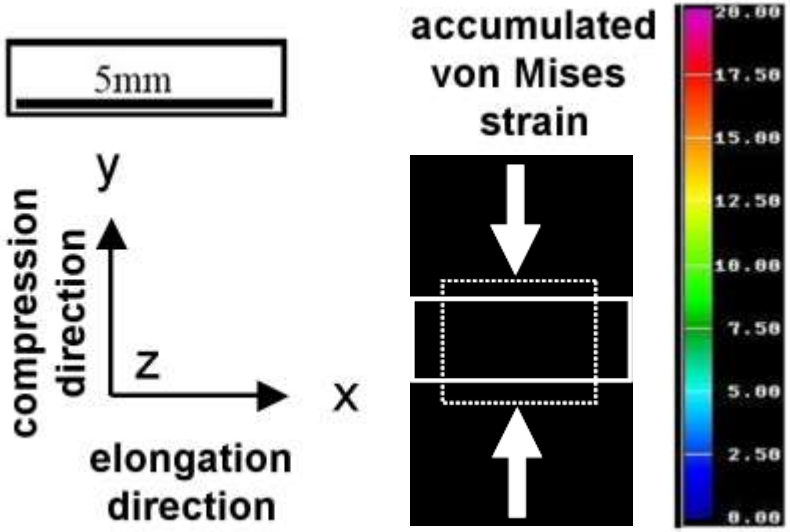
- Examples

Homogeneity and boundary conditions at grain scale

3%



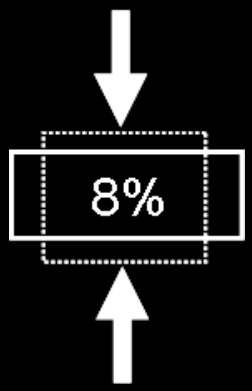


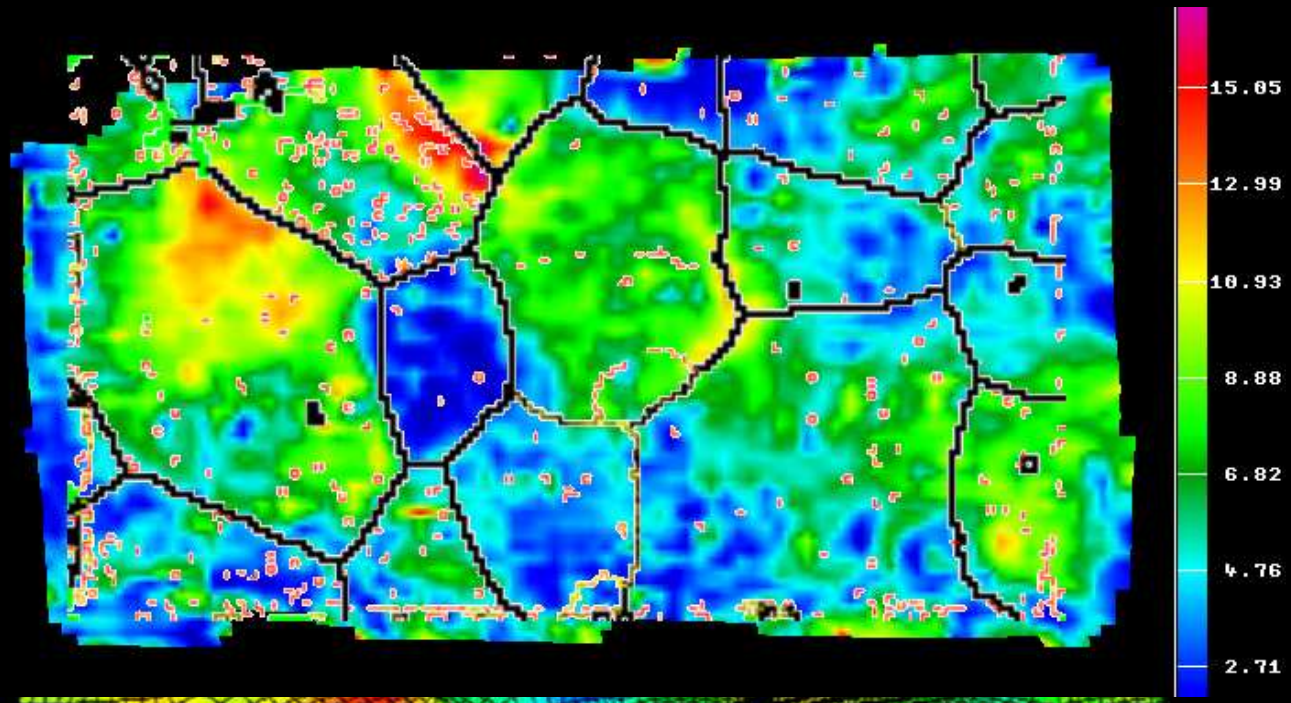


Raabe et al. Acta Mater. 49 (2001) 3433

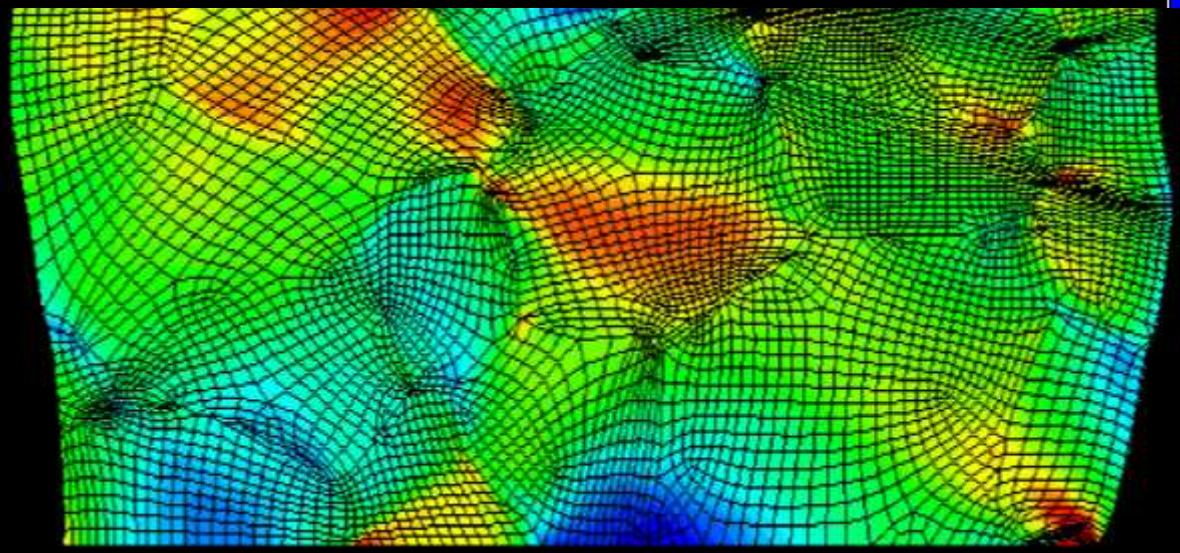
Sachtleber, Zhao, Raabe: Mater. Sc. Engin. A 336 (2002) 81

Crystal Mechanics FEM, grain scale mechanics (2D)

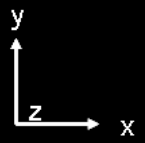




Experiment
(DIC, EBSD)
v Mises strain

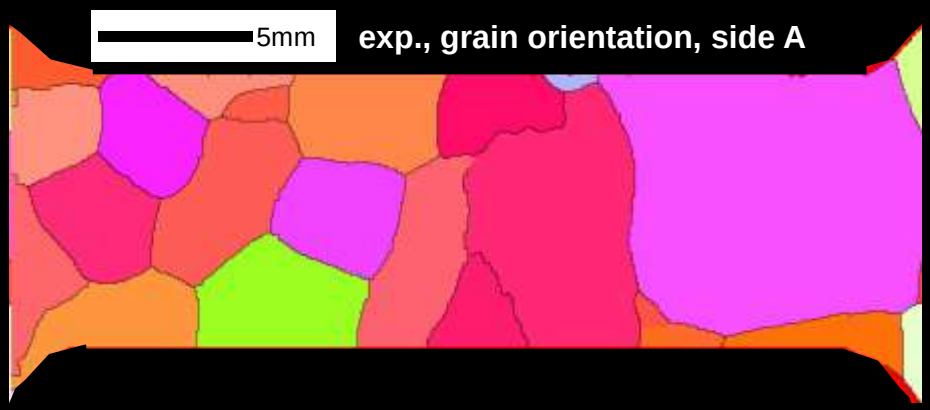


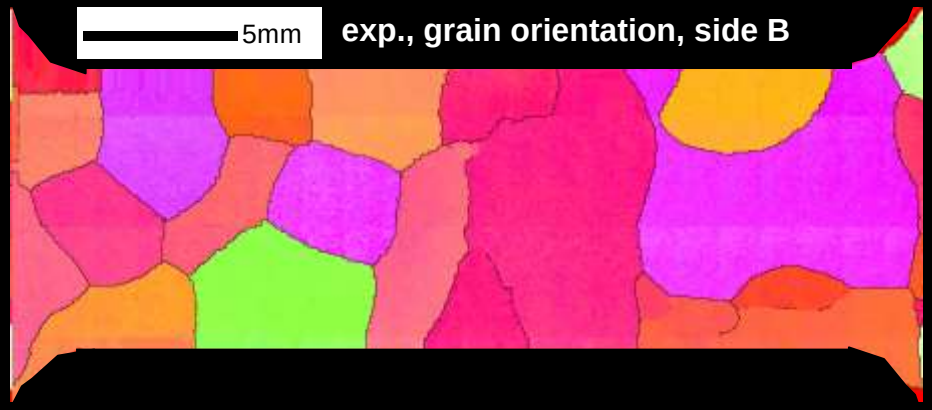
Simulation
(CP-FEM)
v Mises strain

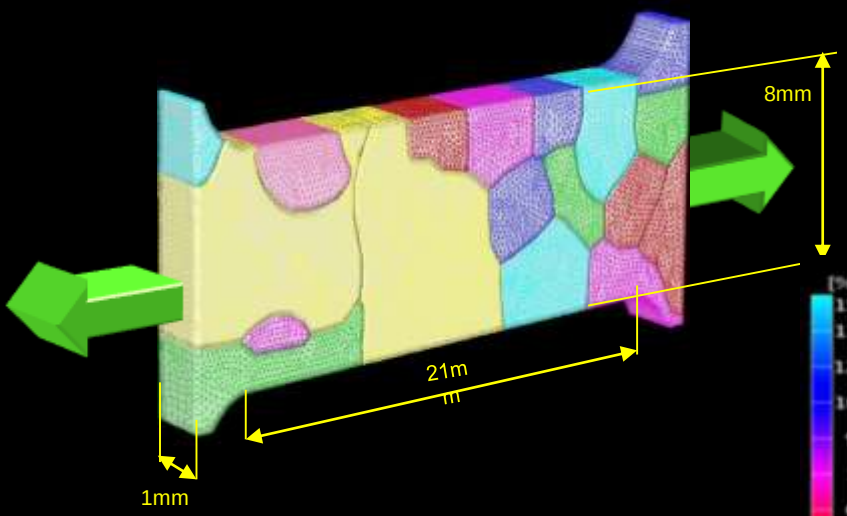


Sachtleber, Zhao, Raabe: Mater. Sc. Engin. A 336 (2002) 81

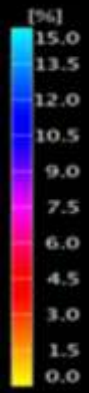
Crystal plasticity FEM, grain scale mechanics (3D Al)

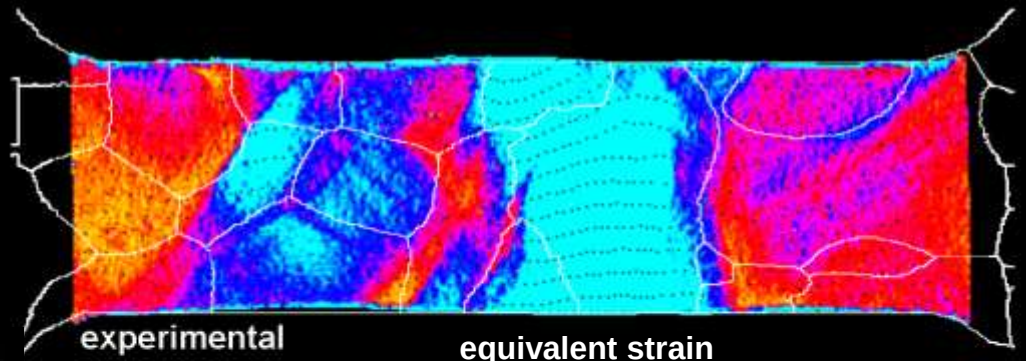


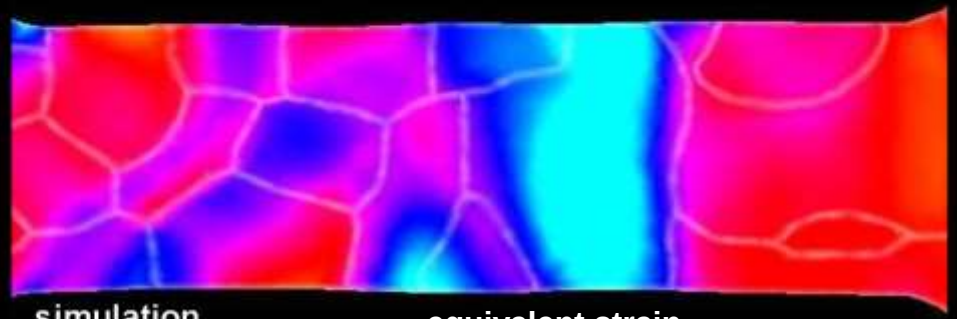




FE mesh

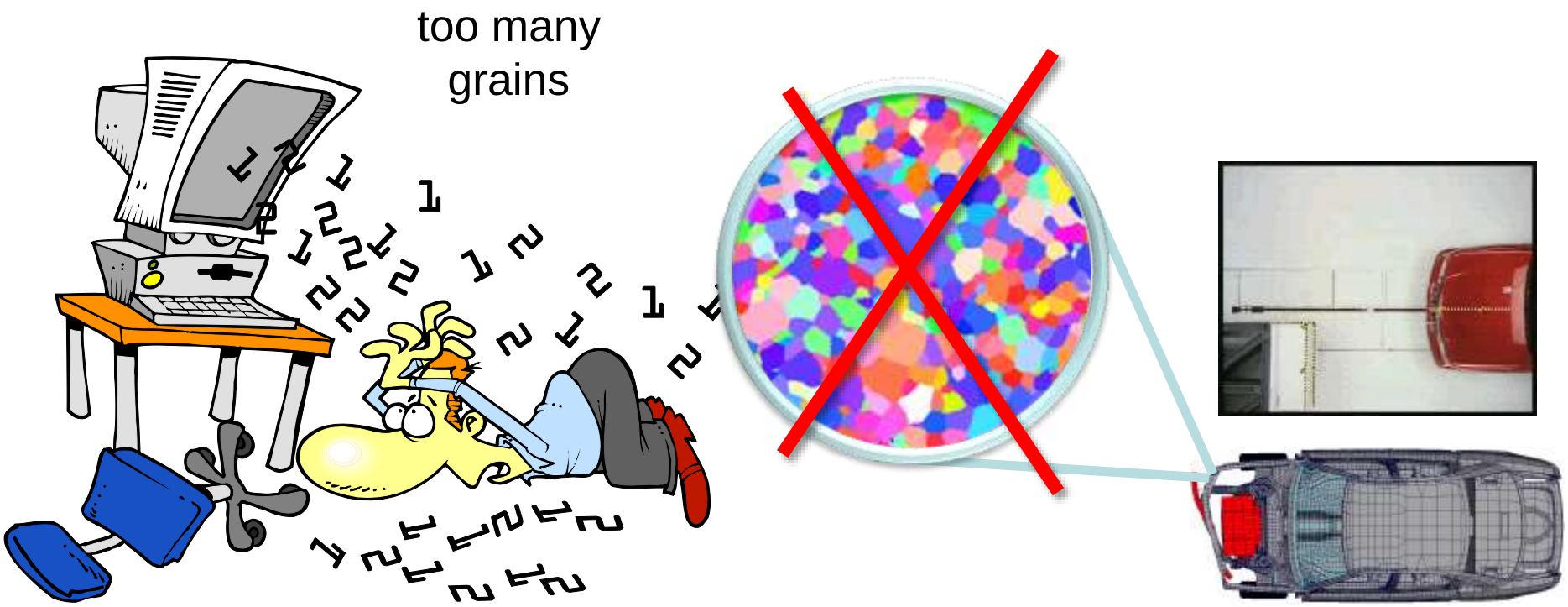






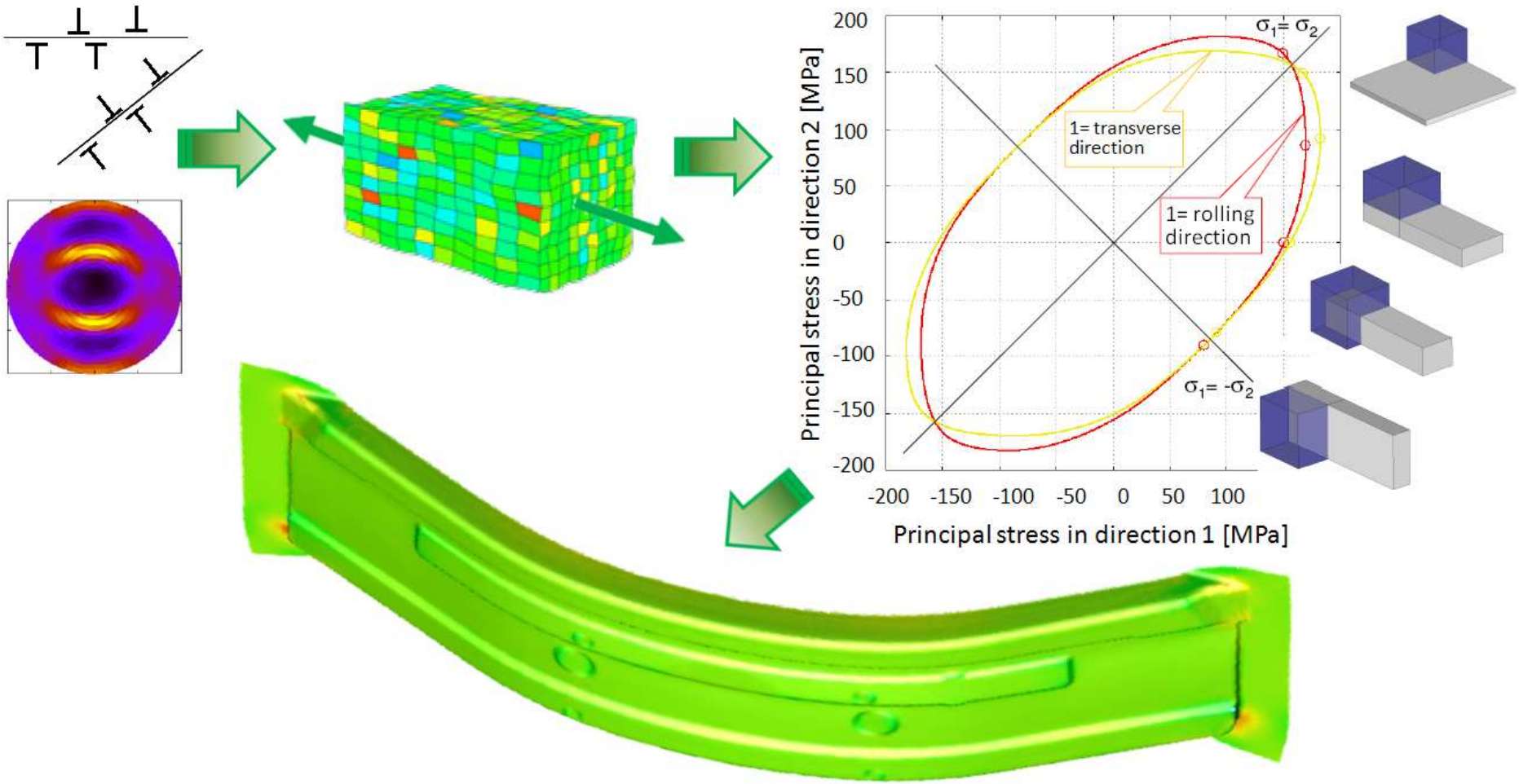
Zhao, Rameshwaran, Radovitzky, Cuitino, Roters, Raabe : Intern. J. Plast. 24 (2008)

Crystal plasticity FEM for large scale forming predictions



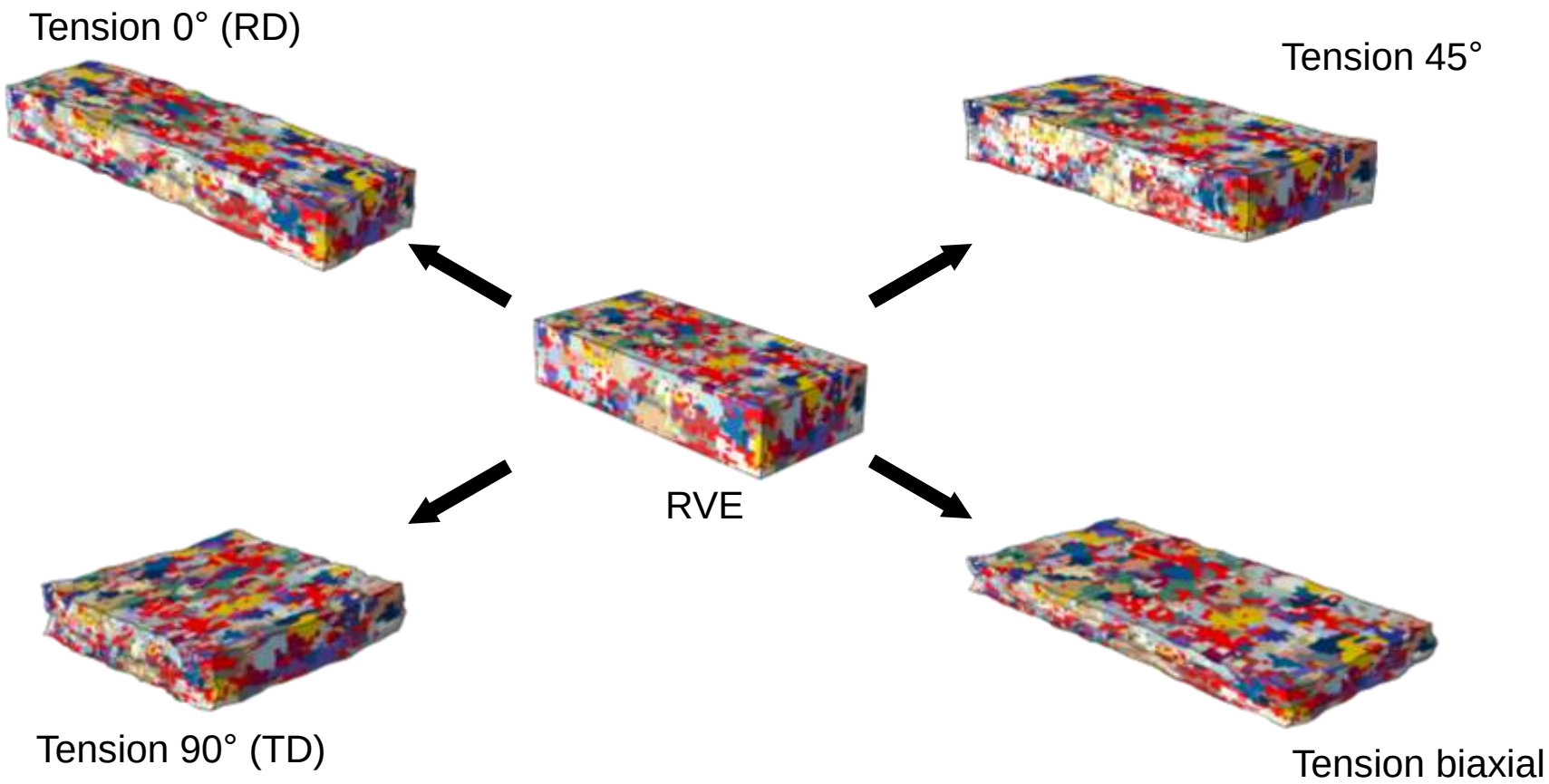
D. Raabe: Advanced Materials 14 No. 9 (2002) p. 639

Numerical Laboratory: From CPFEM to yield surface (engineering)

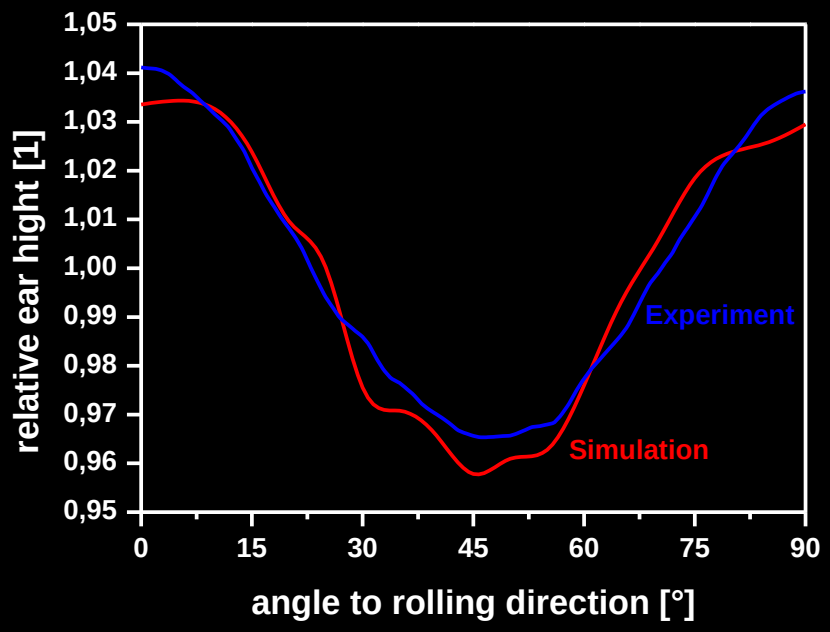


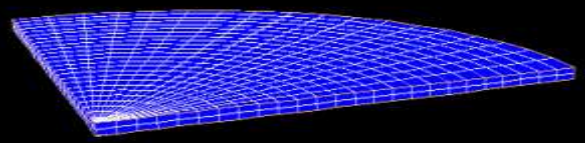
Kraska, Doig, Tikhomirov, Raabe, Roters, Comp. Mater. Sc. 46 (2009) 383

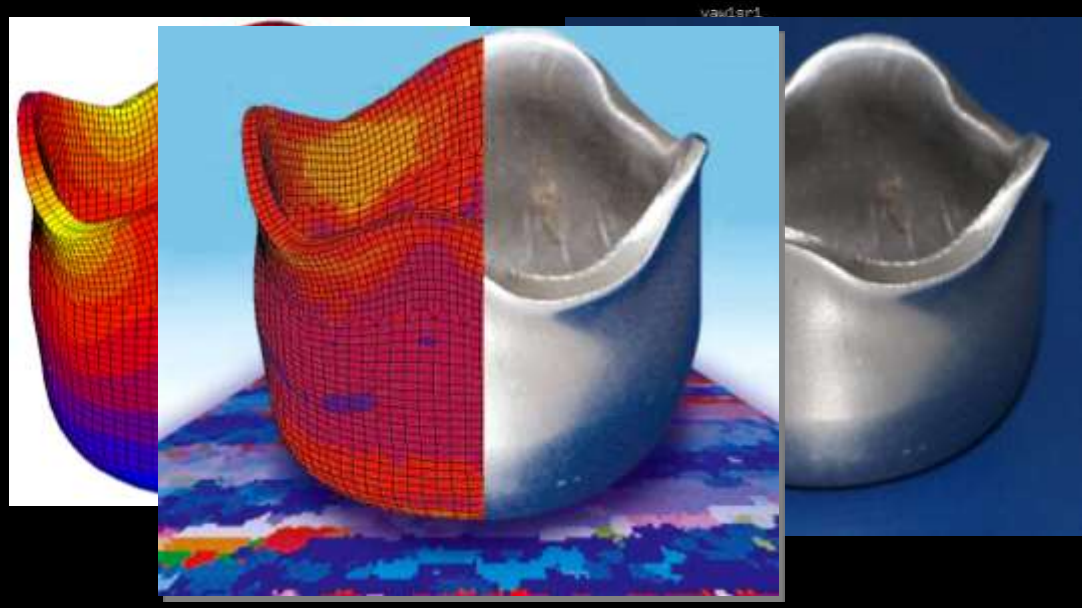
Representative Volume Element



Texture component crystal plasticity FEM for large scale forming

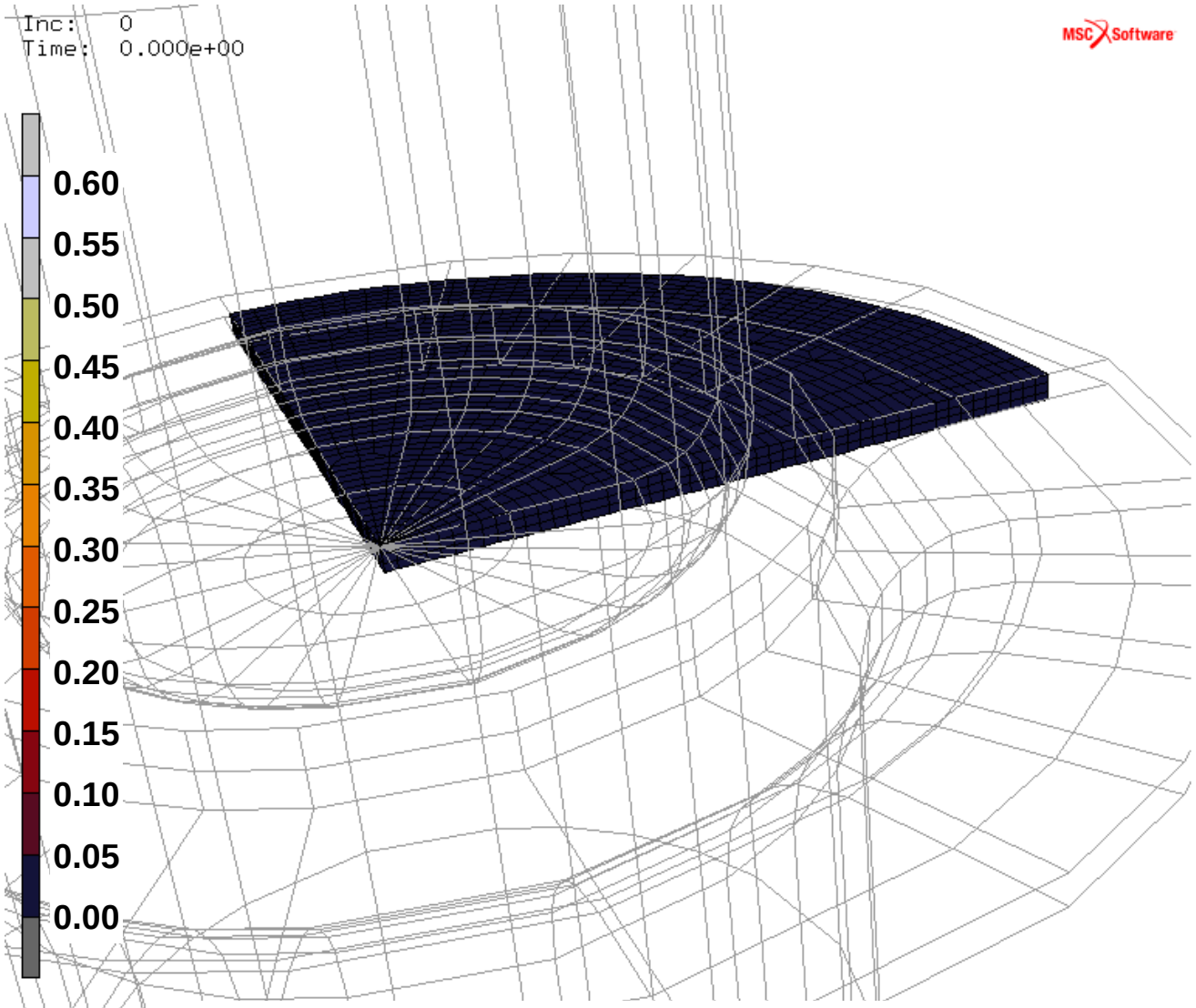






D. Raabe and F. Roters: Intern. J. Plast. 20 (2004) 339

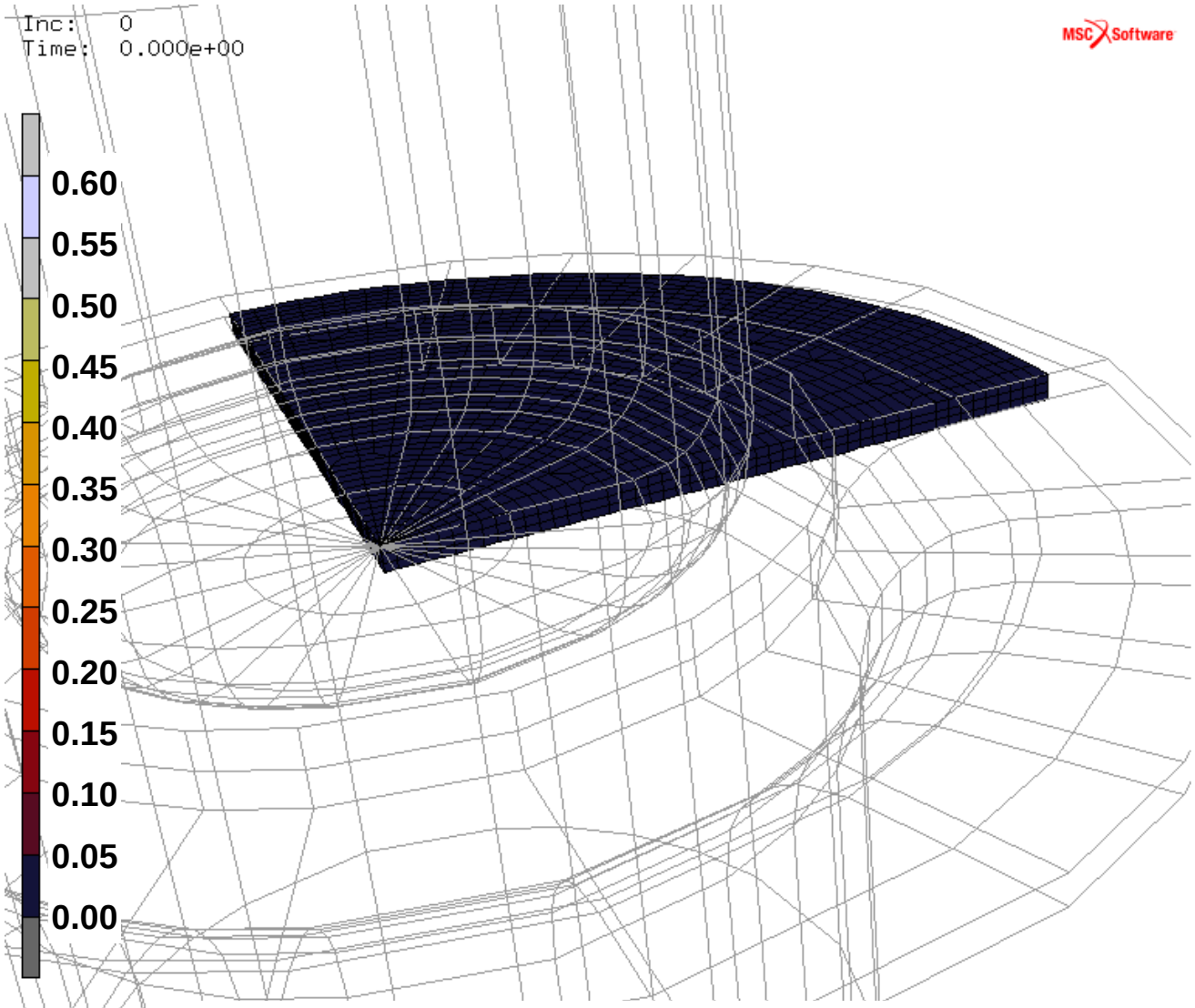
Simulation result: Taylor model



Color map: Equivalent total strain

Roters et al. Acta Mater.58 (2010)

Simulation result: RGC scheme



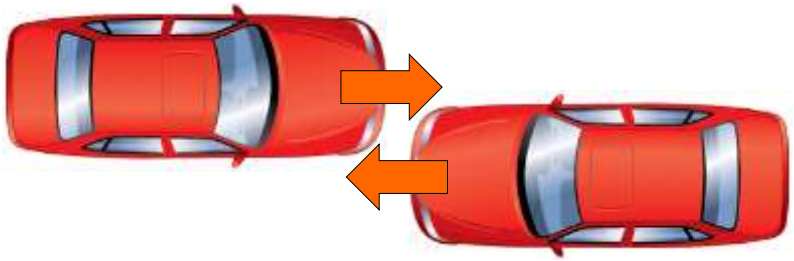
Color map: Equivalent total strain

Roters et al. Acta Mater.58 (2010)

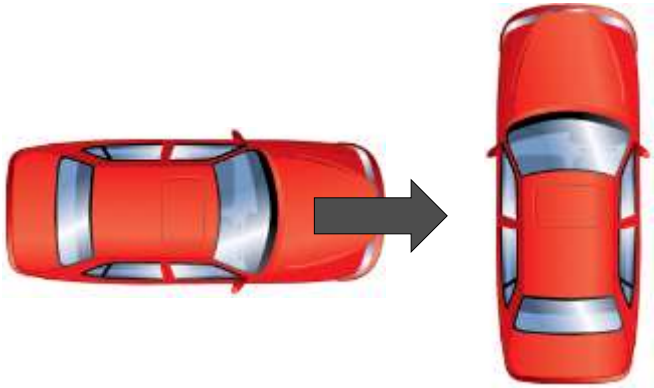
Mechanical properties: ... for which structural component ?

Component-specific property mix

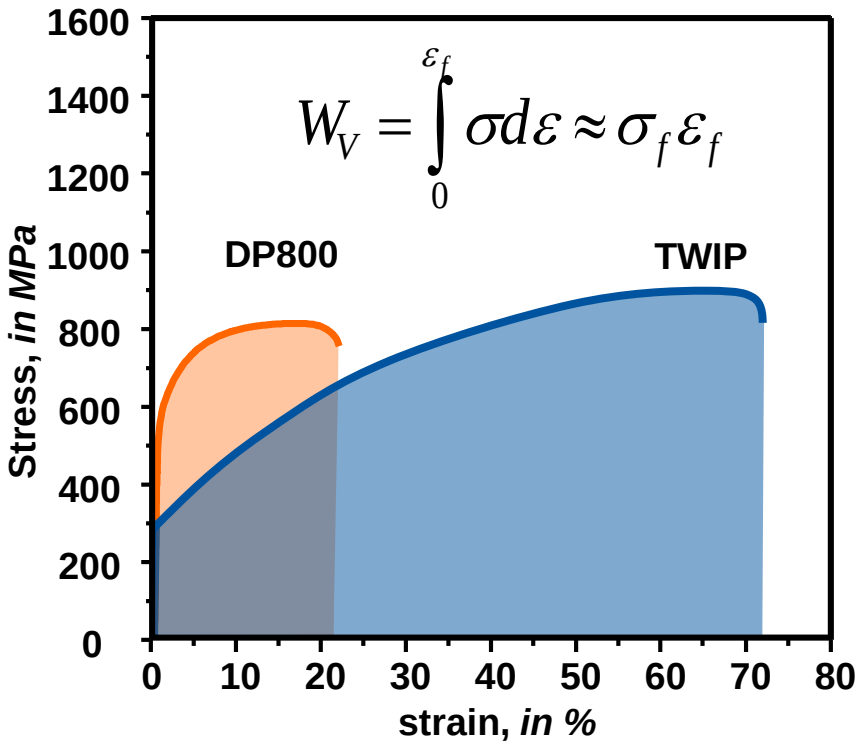
Front crash ⇨ Energy absorption



Side crash ⇨ Strength



Strain rate 800/s: compare TWIP steel to DP800

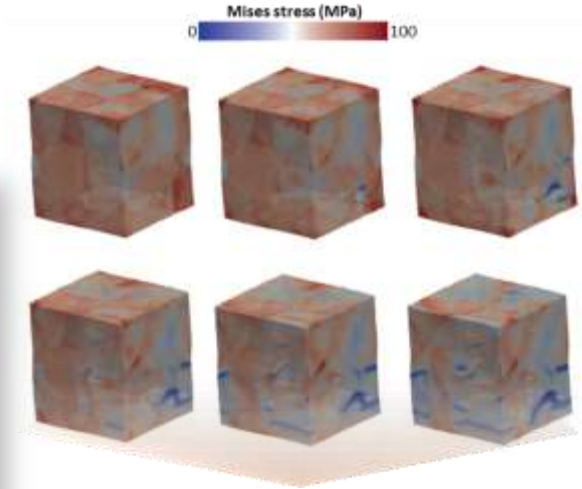


Awareness of impact situation

Düsseldorf Advanced MAterial Simulation Kit, DAMASK

DAMASK
Düsseldorf Advanced Material Simulation Kit
Freeware, GPL 3

Crystal plasticity & phase field:
Mechanics, damage, phase transformation, diffusion



> 15 years of development

> 50 man years of expertise

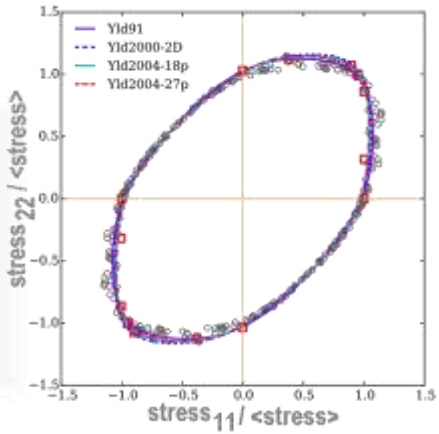
> 50.000 lines of code

Pre- and post-processing

Blends with MSC.Marc and Abaqus

Standalone (FFT) spectral solver

Many user groups



http://DAMASK.mpie.de