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

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Class 2016

class times

Friday, 10 am – 2 pm at IMM / RWTH

(class at MPI Düsseldorf: 17. June 2016)

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

Notes at:

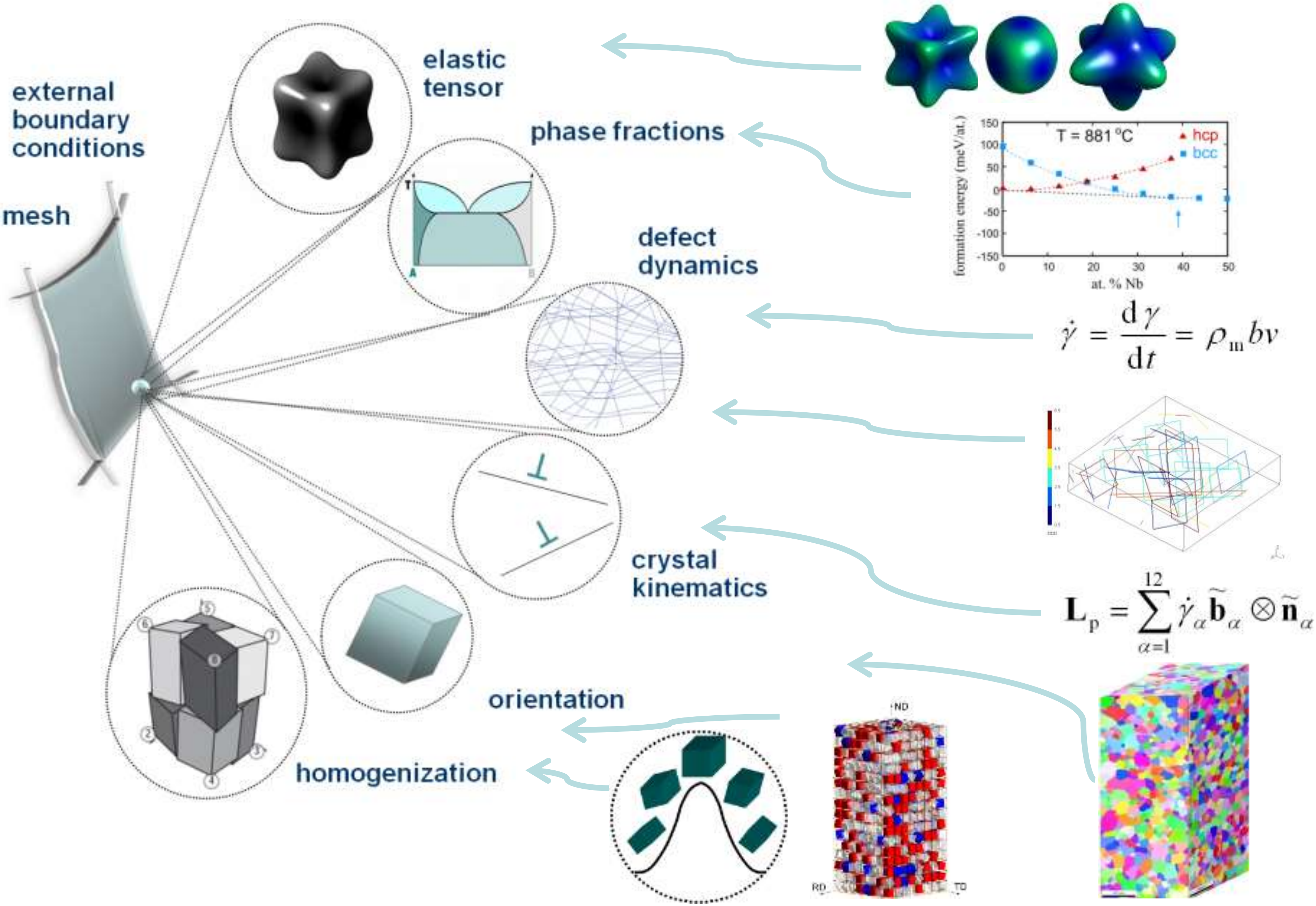
http://www.dierk-raabe.com/teaching/

Homework ?

Contact, website and class days

Date / Location	Topics	Lecturer
15. April 2016 IMM / RWTH	Introduction to materials micromechanics, multiscale problems in micromechanics, case studies, crystal structures and defects, relation to products and manufacturing	Raabe
22. April 2015 IMM / RWTH	Crystal structures, dislocation statics, crystal dislocations, dislocation dynamics	Raabe
29. April 2015 IMM / RWTH	Dislocations, crystalline anisotropy and crystal mechanics in hexagonal metals	Sandlöbes
6. May 2015 IMM / RWTH	No classes	-
13. May 2015 IMM / RWTH	Fracture mechanics Introduction to FEM	Shanthraj
20. May 2015 IMM / RWTH	Athermal phase transformations in micromechanics	Wong
27. May 2015 IMM / RWTH	No classes	-
3. June 2015 IMM / RWTH	Crystal micromechanics, single crystal mechanics, yield surface mechanics, polycrystal models, Taylor model, Integrated micromechanical experimentation and simulation for complex alloys, hydrogen embrittlement	Raabe
10. June 2015 IMM / RWTH	Micromechanics of polymers and biological (natural) composites	Raabe
17. June 2015 MPI / Düsseldorf	!! Class at MPI !! Applied micromechanics: multiphase and composite material design MPI Lab tour	Springer

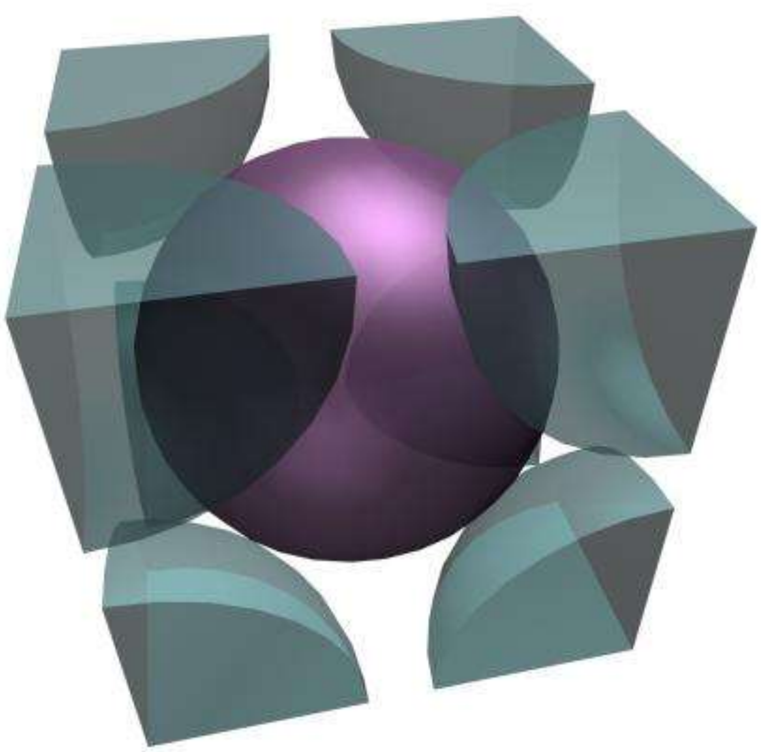
Multiscale crystal plasticity FEM



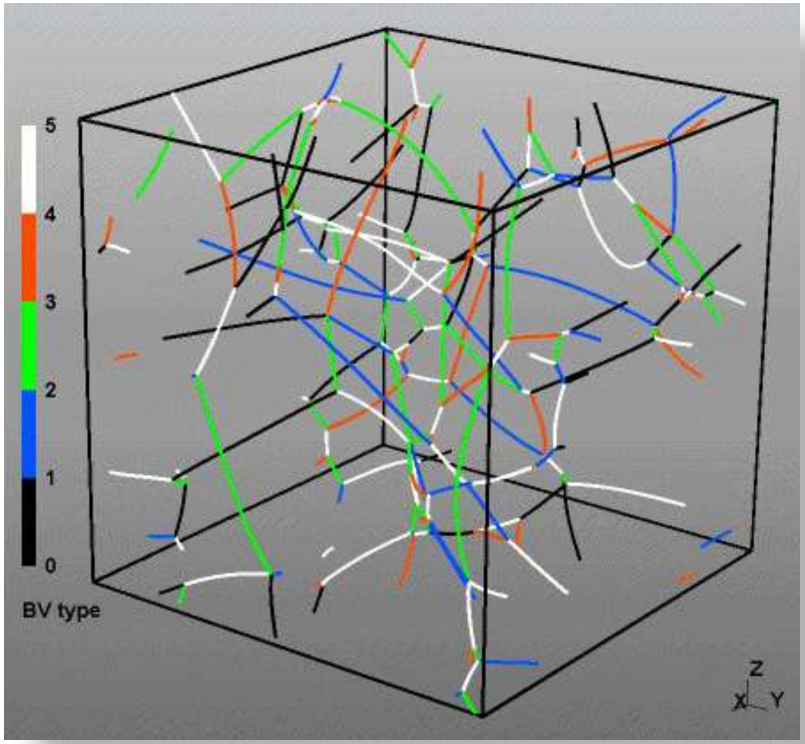
Raabe, Zhao, Park, Roters: Acta Mater. 50 (2002) 421

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



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

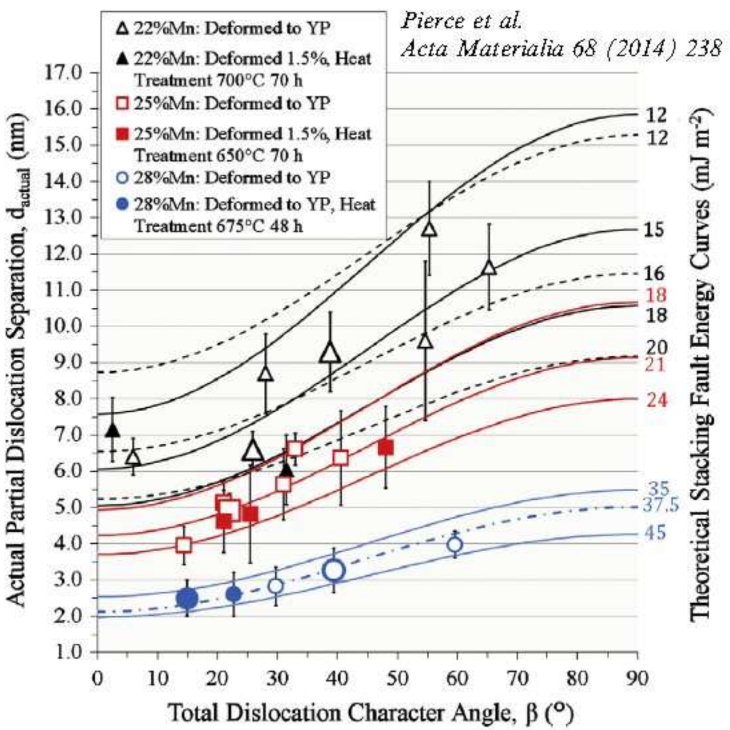
Shockley partial dislocations (b = a/6<112>)

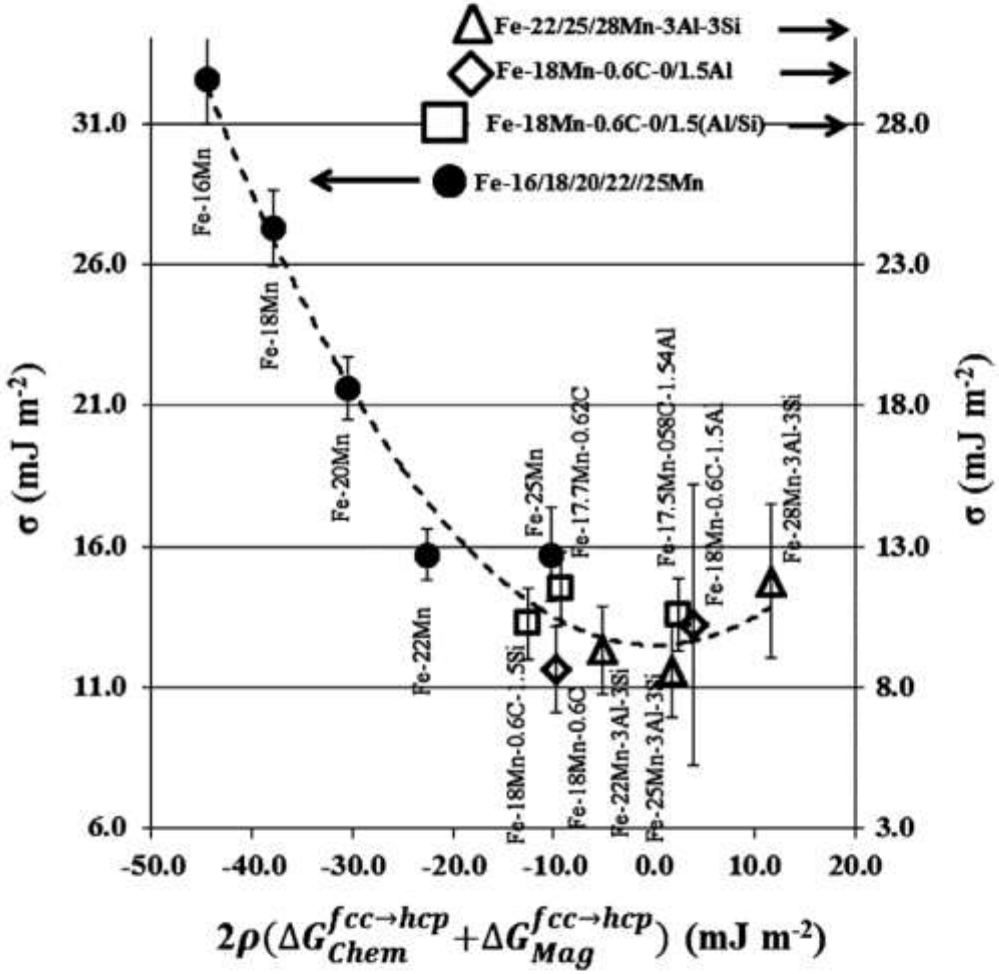
Special properties of the 3 main lattice types regarding plasticity defects

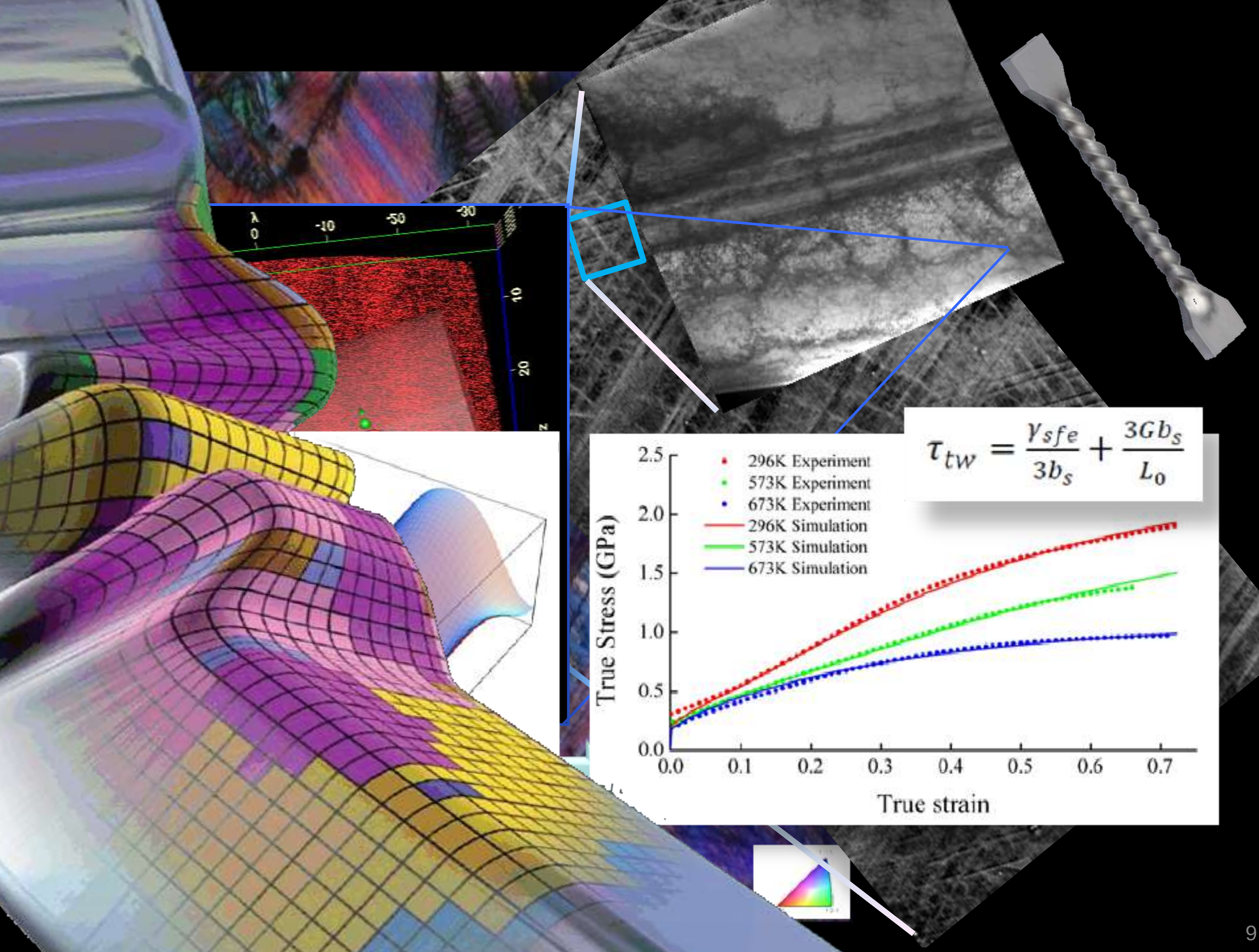
FCC: stacking fault energy can vary from very low values (α-Brass- 30 wt% Zn in Cu; TWIP steels: ≈ 20 mJ/m²) to very high values (Al : ≈ 180 mJ/m²): Regarding lattice defects in plasticity FCC and hcp is not a 'homogeneous' or unique crystal structure

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

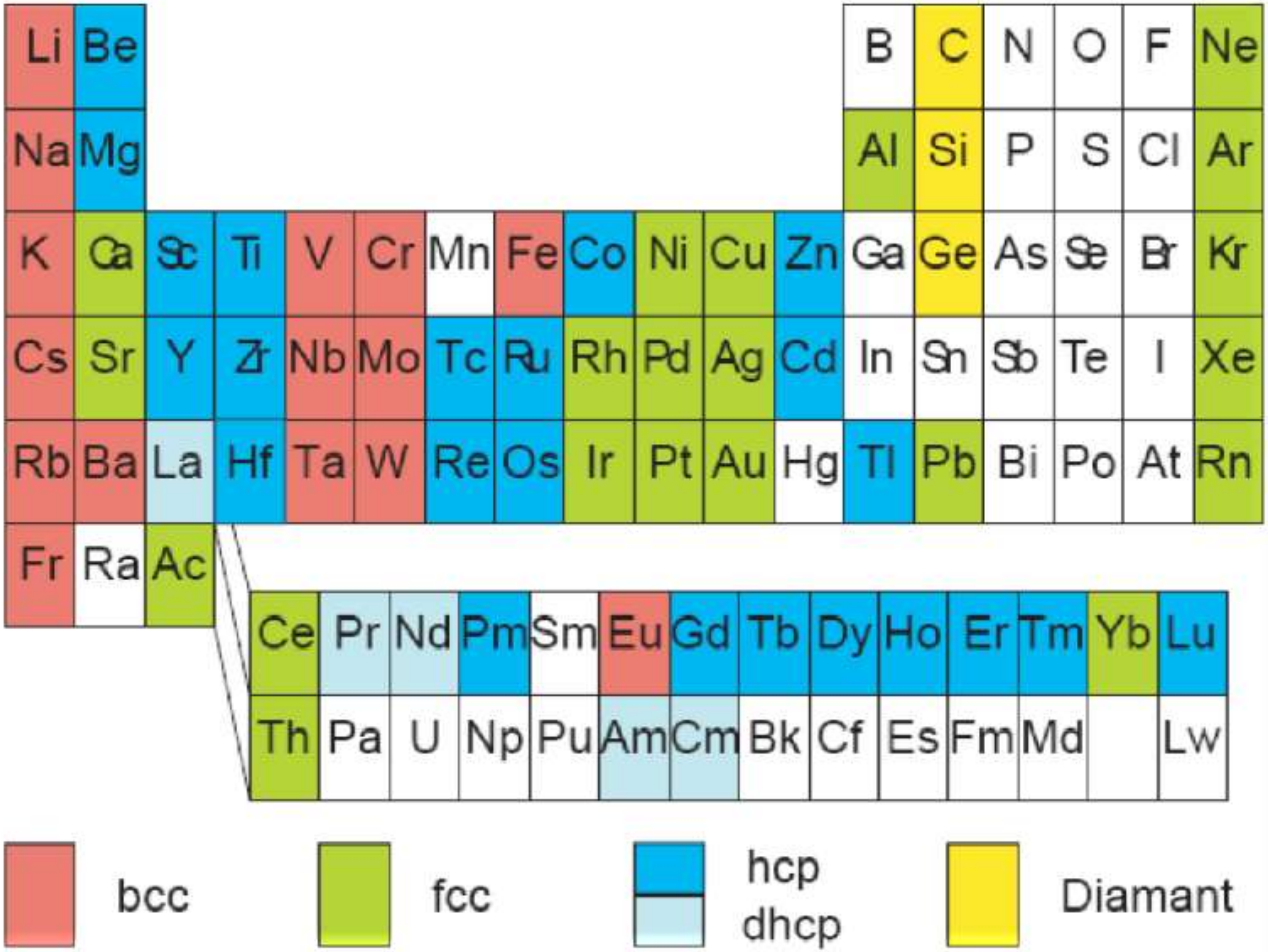

Pierce et al.
Acta Materialia 68 (2014) 238
22%Mn: Deformed to YP
22%Mn: Deformed 1.5%, Heat Treatment 700°C 70 h
25%Mn: Deformed to YP
25%Mn: Deformed 1.5%, Heat Treatment 650°C 70 h
28%Mn: Deformed to YP
28%Mn: Deformed to YP, Heat Treatment 675°C 48 h
Actual Partial Dislocation Separation, d_{actual} (nm)
Theoretical Stacking Fault Energy Curves (mJ m^{-2})
Total Dislocation Character Angle, β (°)


Fe-22/25/28Mn-3Al-3Si
Fe-18Mn-0.6C-0/1.5Al
Fe-18Mn-0.6C-0/1.5(Al/Si)
Fe-16/18/20/22//25Mn
σ (mJ m^{-2})
$2\rho(\Delta G^{fcc\rightarrow hcp}_{Chem} + \Delta G^{fcc\rightarrow hcp}_{Mag})$ (mJ m^{-2})



296K Experiment
573K Experiment
673K Experiment
296K Simulation
573K Simulation
673K Simulation
True Stress (GPa)
True strain
0.0
0.5
1.0
1.5
2.0
2.5
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$\tau_{tw} = \frac{\gamma_{sfe}}{3b_s} + \frac{3Gb_s}{L_0}$

How frequently do certain crystal structures occur in the PSE?



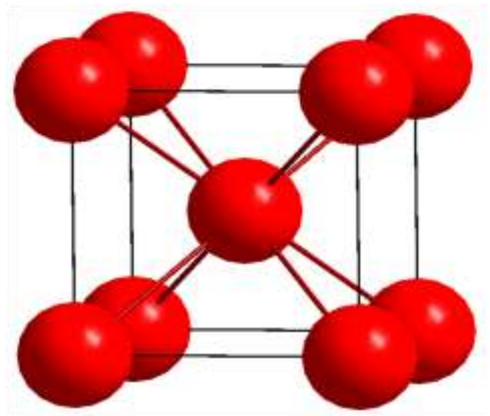
Lattice parameters

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)	

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

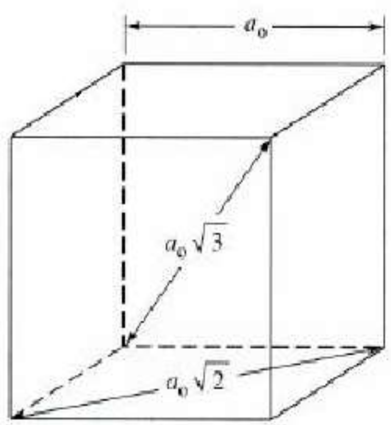
coordination number $= 4 + 4 = 8$

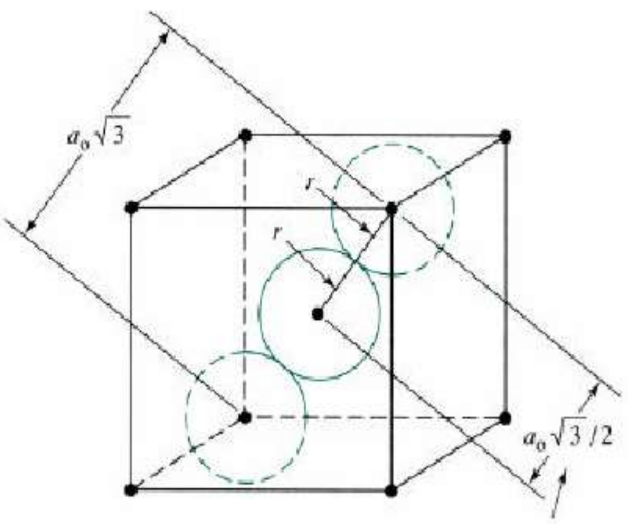
atomic packaging $= 0.68$



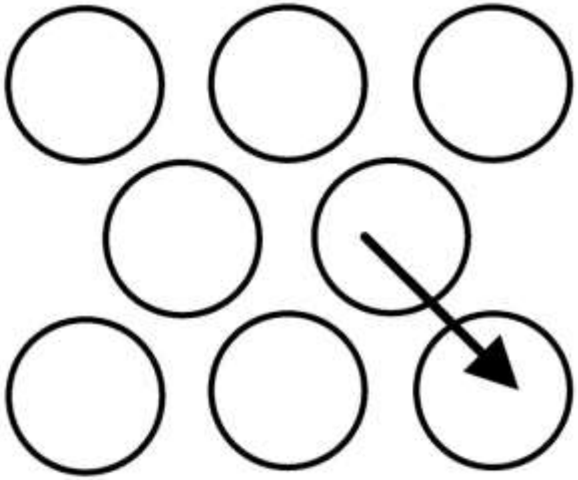
$$4r = \sqrt{3}a$$

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

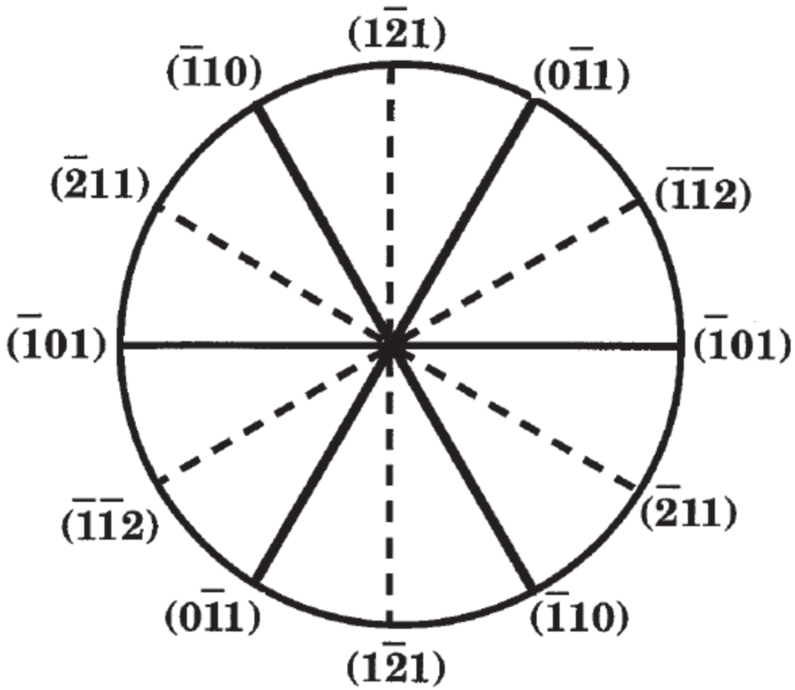




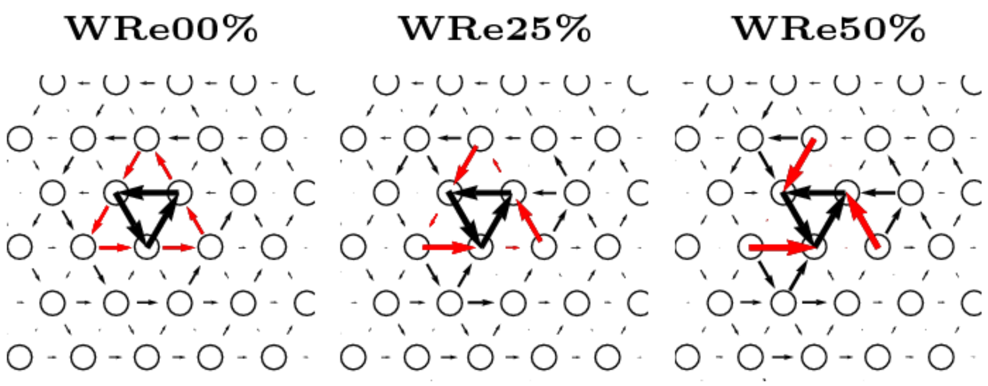
Glide plane: BCC



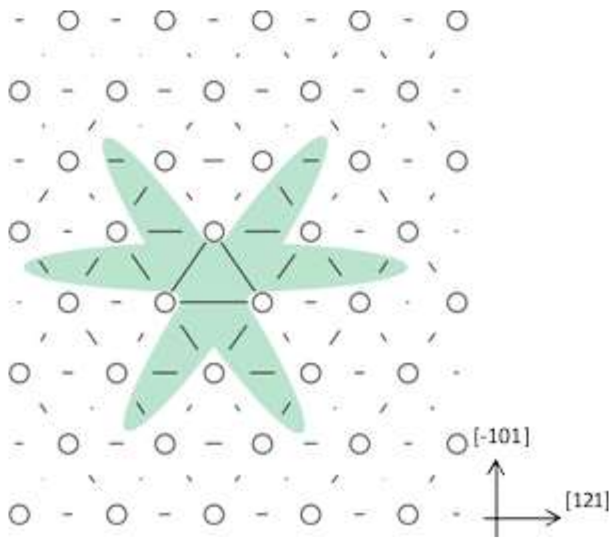
Glide plane: BCC



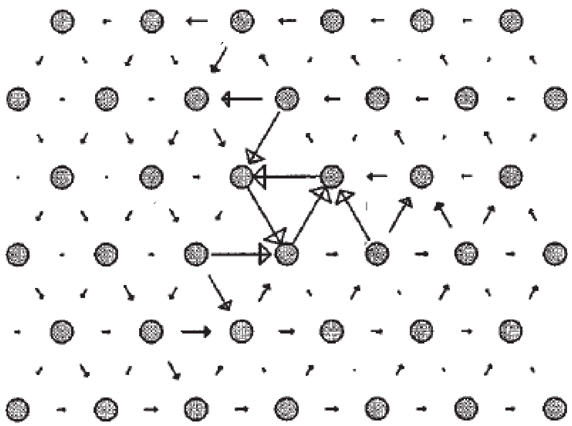
[111] stereographic projection showing orientations of all {110} and {112} planes belonging to the [111] zone.



source: Ambrosch-Draxl



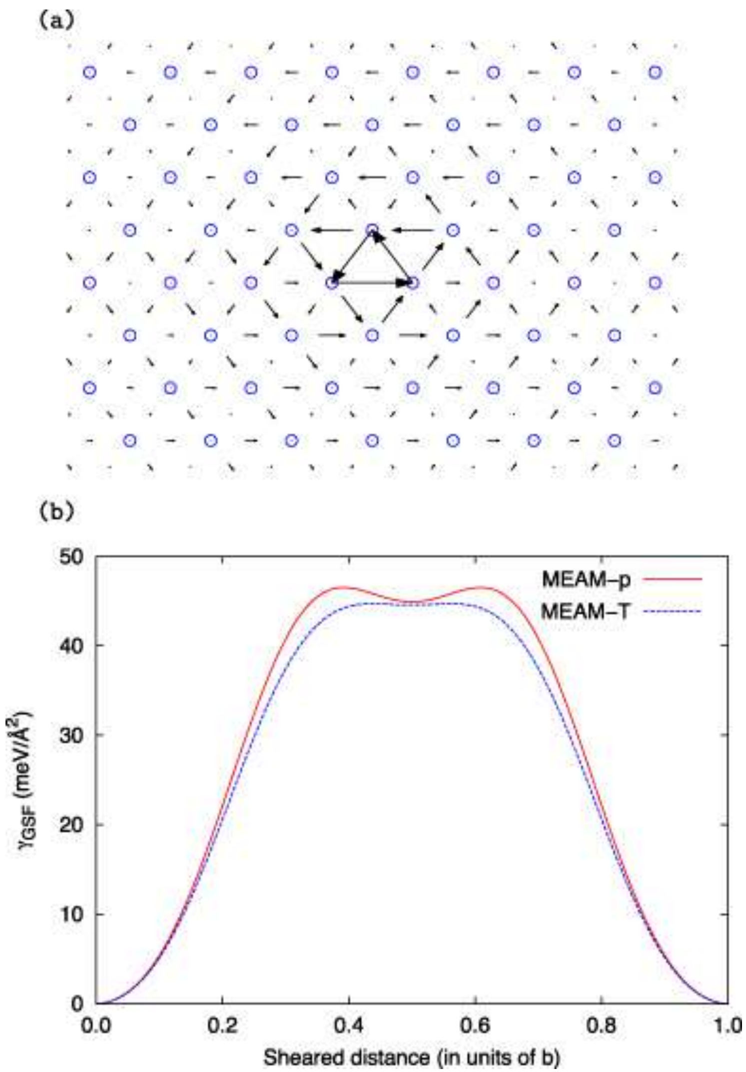
source: ICAMS/RUB



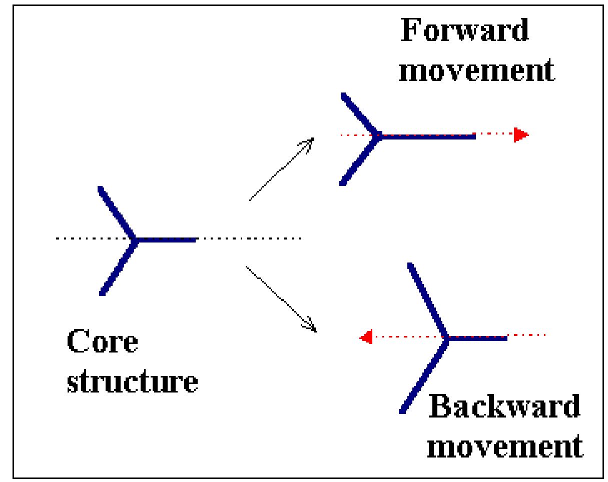
V. Vitek

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

Crystal dislocations: BCC structure



Tongsik Lee et al 2012 J. Phys.: Condens. Matter 24 225404



may lead to non-Schmid behaviour

$$\tau = \sigma_{ij}^{dev} m_{ij}$$

slip system s

n_i^s, b_i^s

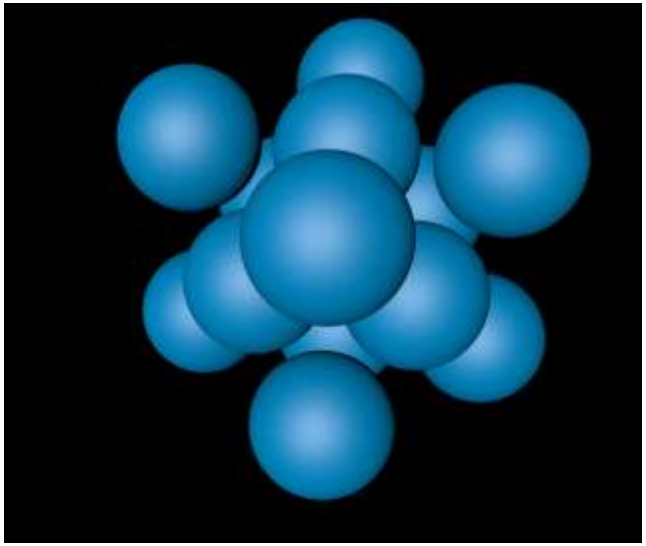
$$\tau = \sigma_{ij}^{dev+hydr} m_{ij}$$

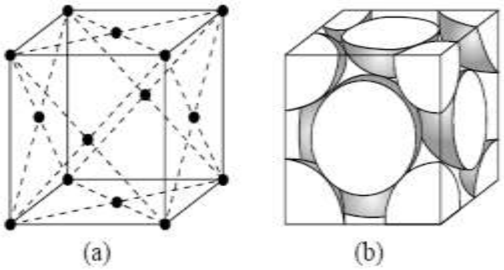
orientation factor for s

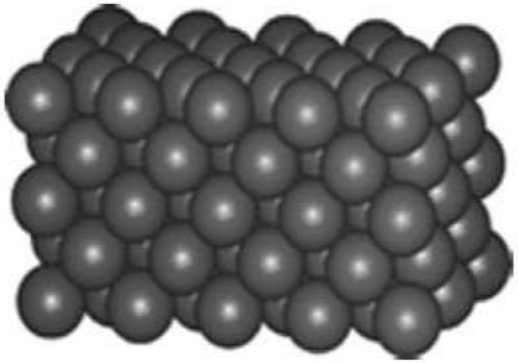
$m_{ij}^s = n_i^s b_j^s$

Perfect screw: no fixed glide plane
real screw: due to the asymmetry between forward and backward motion, there is a certain probability that screw dislocation switches glide planes

Fe (γ), Al, Cu, Au



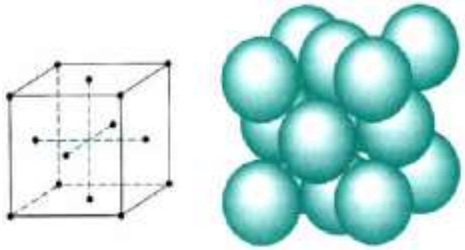




atoms per cell = (8 x 1/8) + (6 x ½) = 4

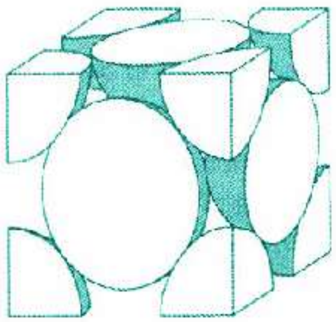
coordination number = 4 + 4 + 4 = 12

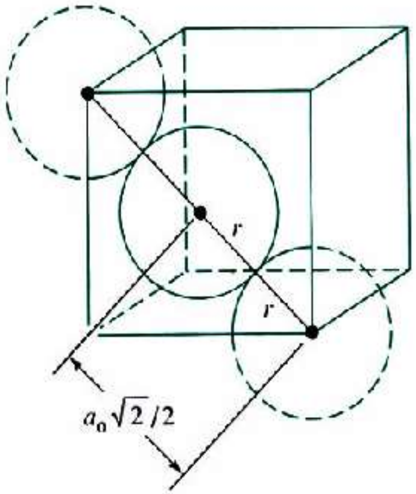
atomic packaging = 0.74



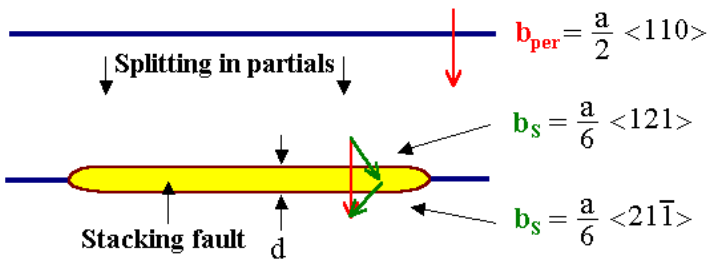
$$4r = \sqrt{2}a$$

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



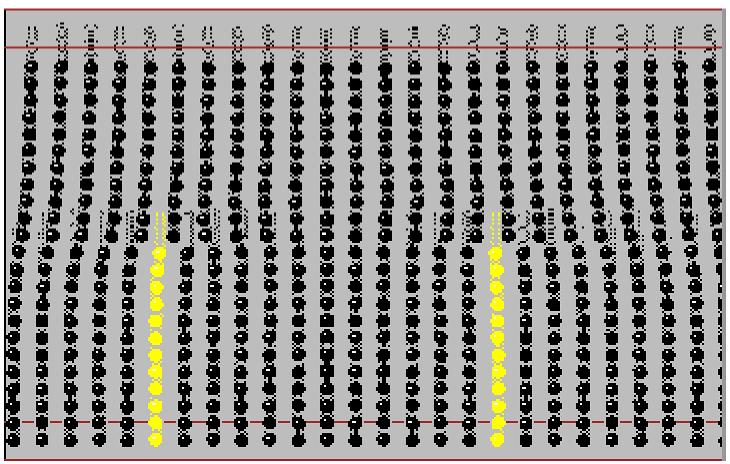


Crystal dislocations: FCC structure

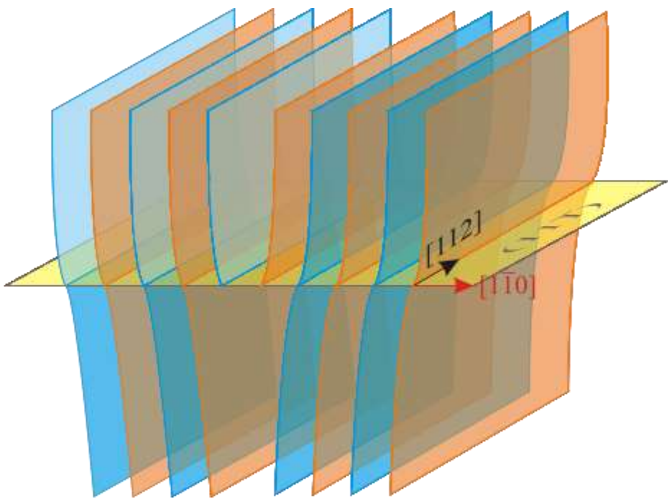


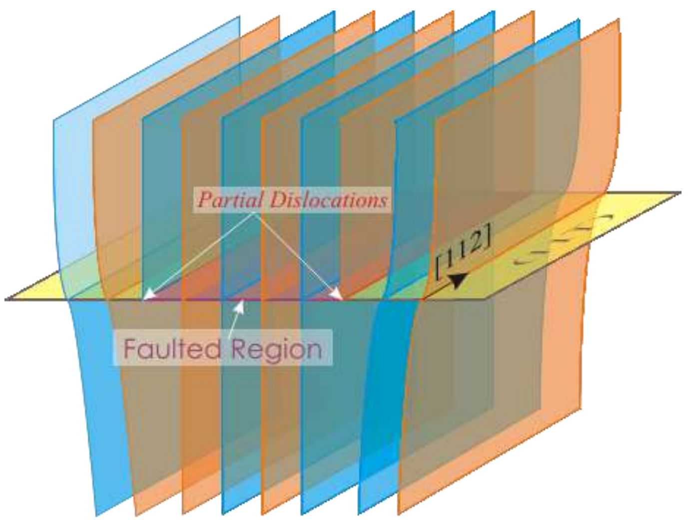
Energy of the perfect dislocation $= G \cdot b^2 = G \cdot (a/2<110>)^2 = \dfrac{G \cdot a^2}{2}$

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

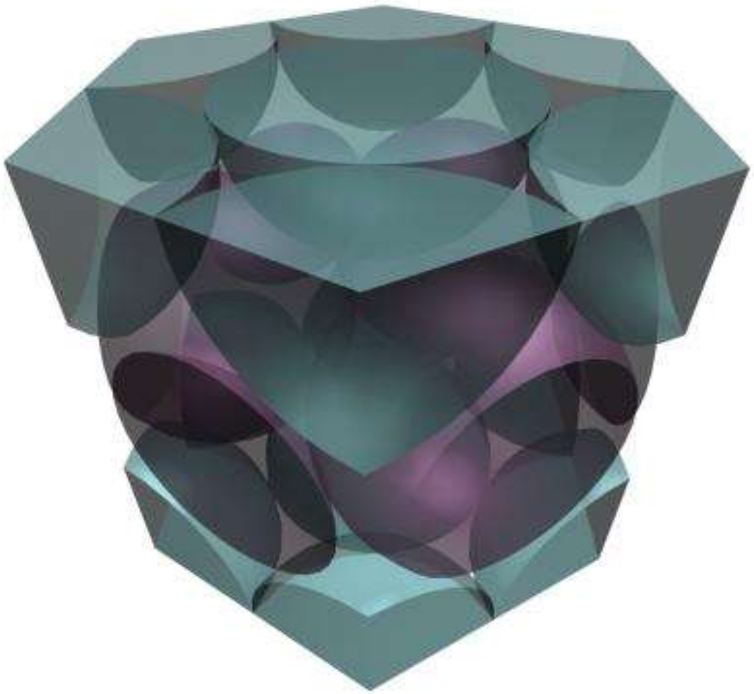


L. Perondi, M. Robles, K. Kaski, and A. Kuronen





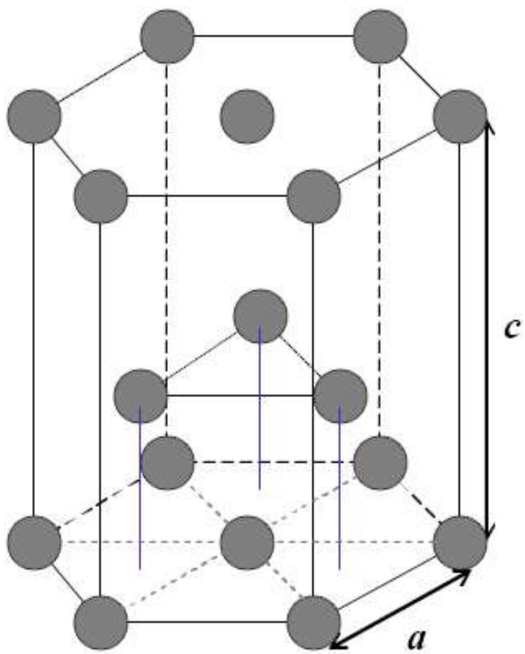
Crystal structure: Hexagonal

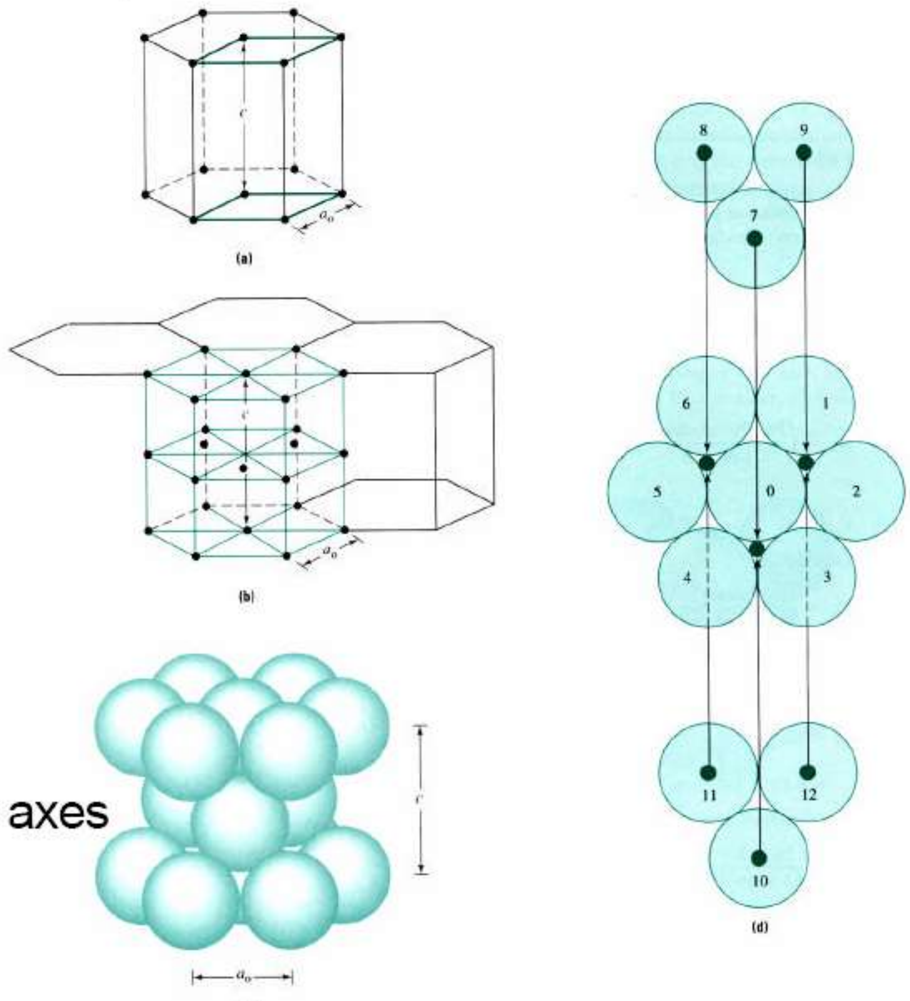


Seperate class by Dr. Sandlöbes

3. HCP: hexagonal close-packed

(Mg, Be, Co, Ti, Zn)

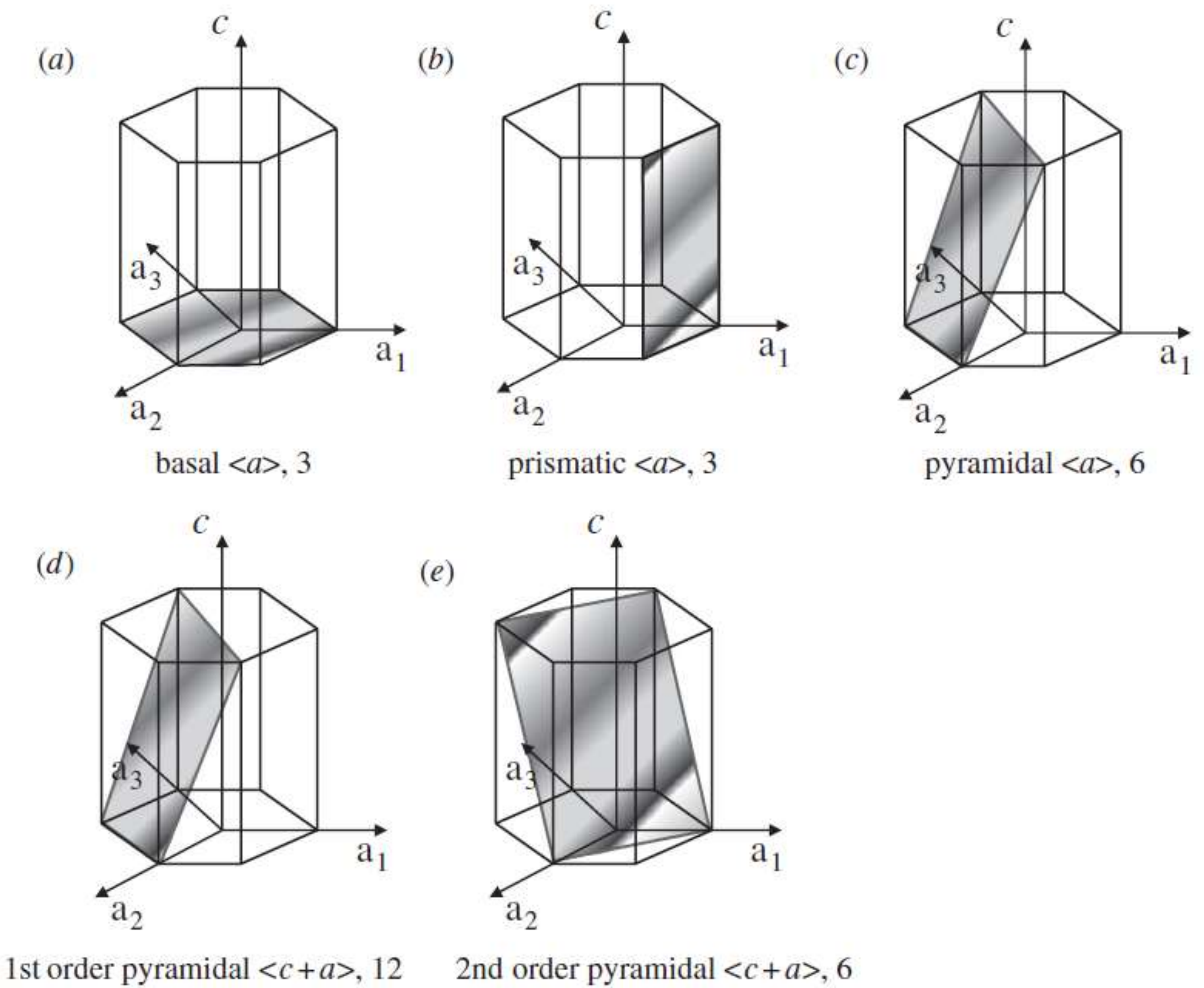




noncubic symmetry: ***a*** and ***c*** axes

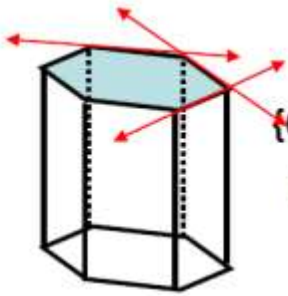
c/a ~ 1.633

Crystal structure: Hexagonal



HCP Slip Planes and Directions

Principal slip system can depend on c/a and *relative orientation of load to slip planes*

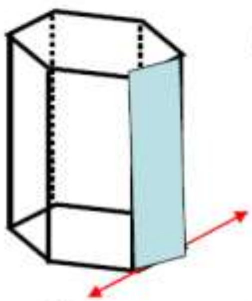


{0001} planes in the direction of $\langle 11\bar{2}0 \rangle$

Slip systems: 1 x 3 = 3

c/a ≥ 1.6333 (ideal)

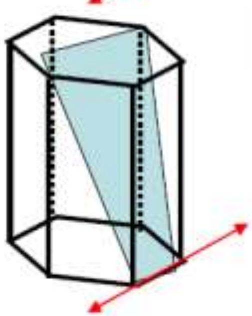
Cd, Zn, Mg, Ti, Be ...



$\{10\bar{1}0\}$ planes in the direction of $\langle 11\bar{2}0 \rangle$

Slip systems: 3 x 1 = 1

Ti



$\{10\bar{1}1\}$ planes in the direction of $\langle 11\bar{2}0 \rangle$

Slip systems: 6 x 1 = 6

c/a ≤ 1.6333 (ideal)

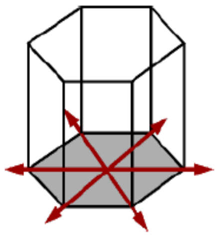
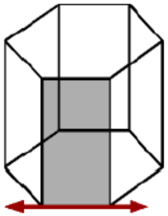
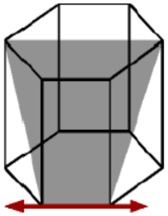
Mg, Ti

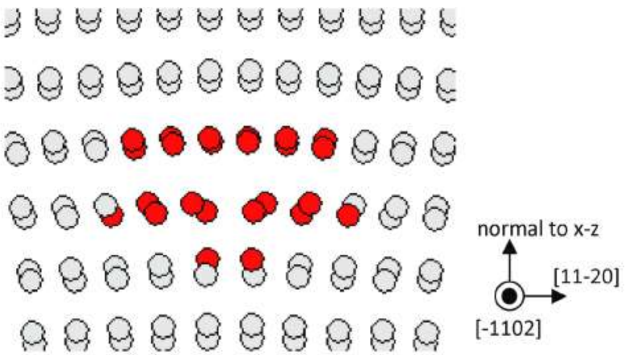
hcp Zinc single crystal

Adapted from Fig. 7.9, *Callister 6e.*

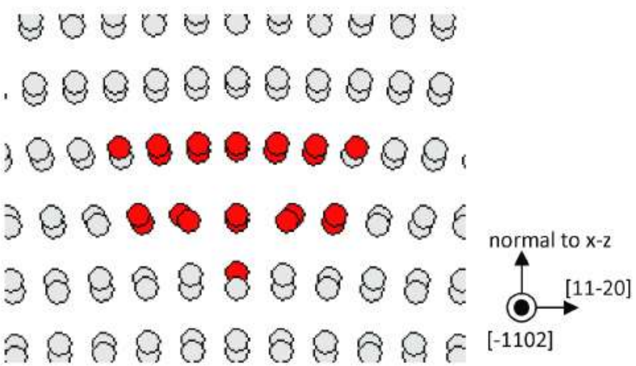
Adapted from Fig. 7.8, *Callister 6e.*

vectors and planes for hexagonal materials

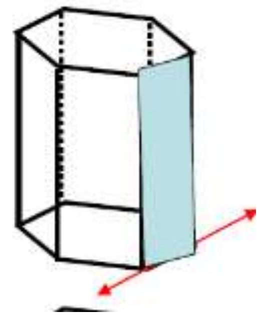
Gitter	Beispiel		Gleitebenen G Typ	Gleitebenen G Zahl	Gleitrichtung g Typ	Gleitrichtung g Zahl	Gesamtzahl der Gleitsysteme
hex	Cd Zn Mg Ti_{α} Be		(0001)	1	[1120]	3	3
	Cd Zn Mg Ti_{α} Be Zr_{α}		(1010)	3	[1120]	1	3
	Mg Ti_{α}		(1011)	6	[1120]	1	6

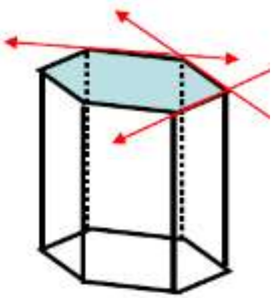


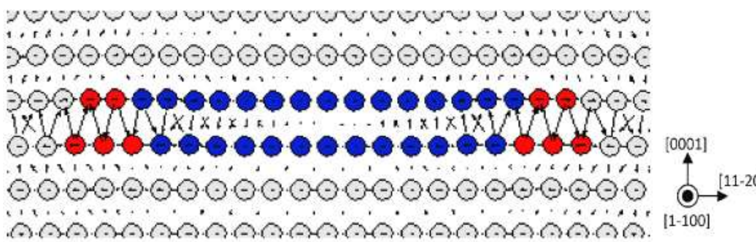
(a) OFDFT/WT/LDA/BLPS (initial separation = 0.0 Å)



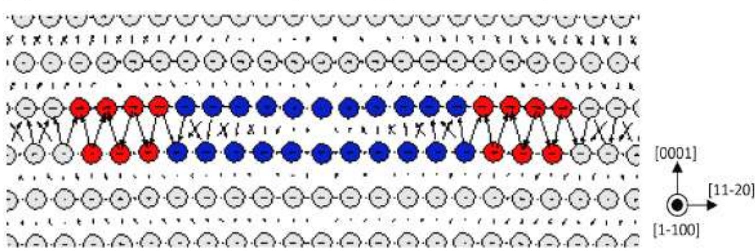
(b) EAM/Sun's (initial separation = 0.0 Å)







(a) OFDFT/WT/LDA/BLPS (initial separation = 0.0 Å)

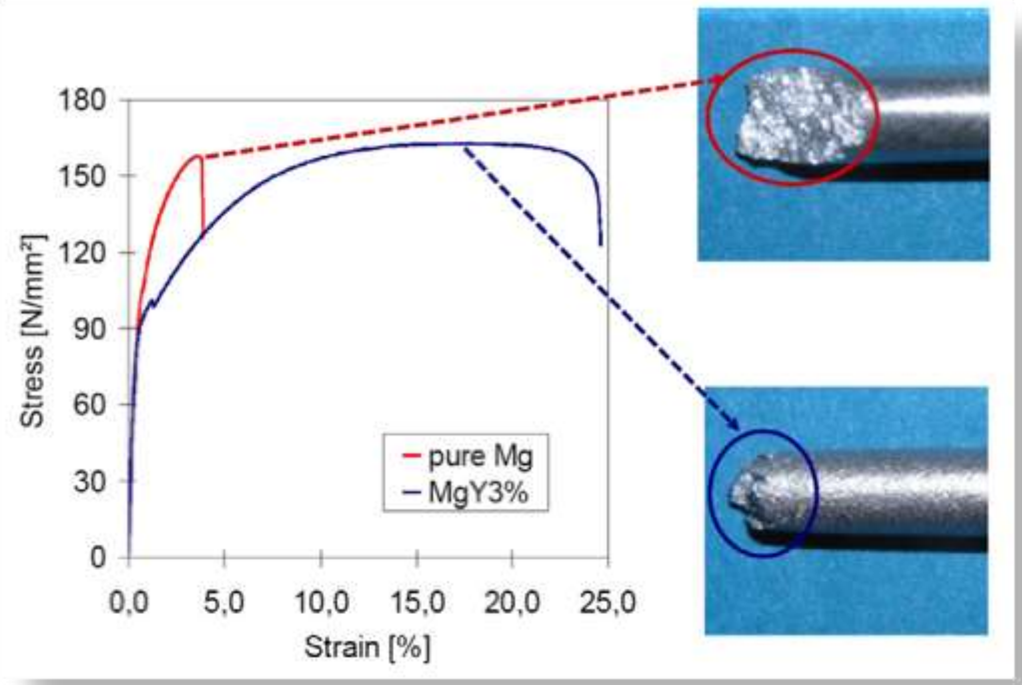


(b) EAM/Sun's (initial separation = 0.0 Å)

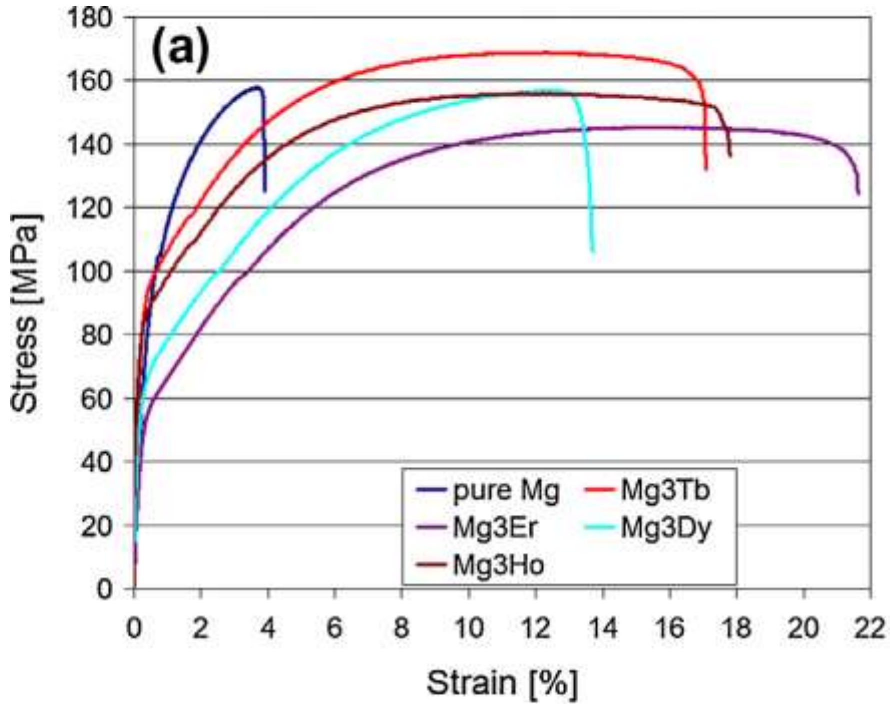
Ilgyou Shin and Emily A Carter 2012 Modelling Simul. Mater. Sci. Eng. 20 015006

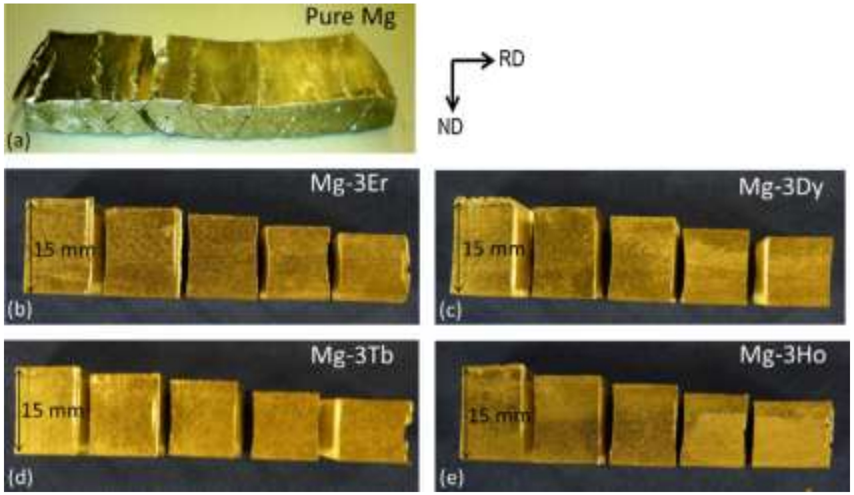
Hex: hcp or hex?; c/a ratio determines slip systems and twinning: some hex metals are very brittle (Mg) and some are rather ductile (Ti)

Mg - RE


180
150
120
90
60
30
0
Stress [N/mm²]
0,0
5,0
10,0
15,0
20,0
25,0
Strain [%]
pure Mg
MgY3%

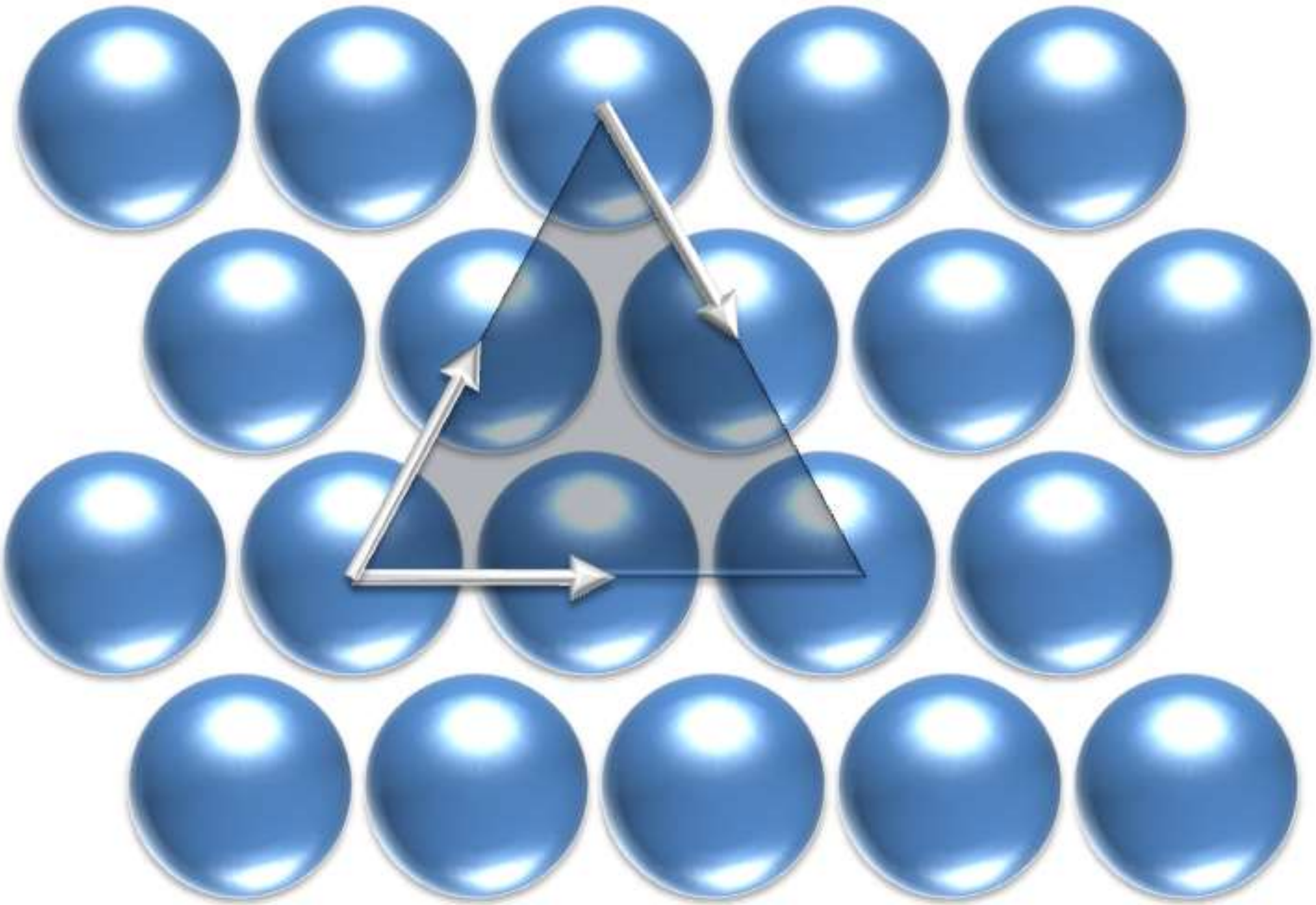
Crystal dislocations: Hex structure – example of Mg



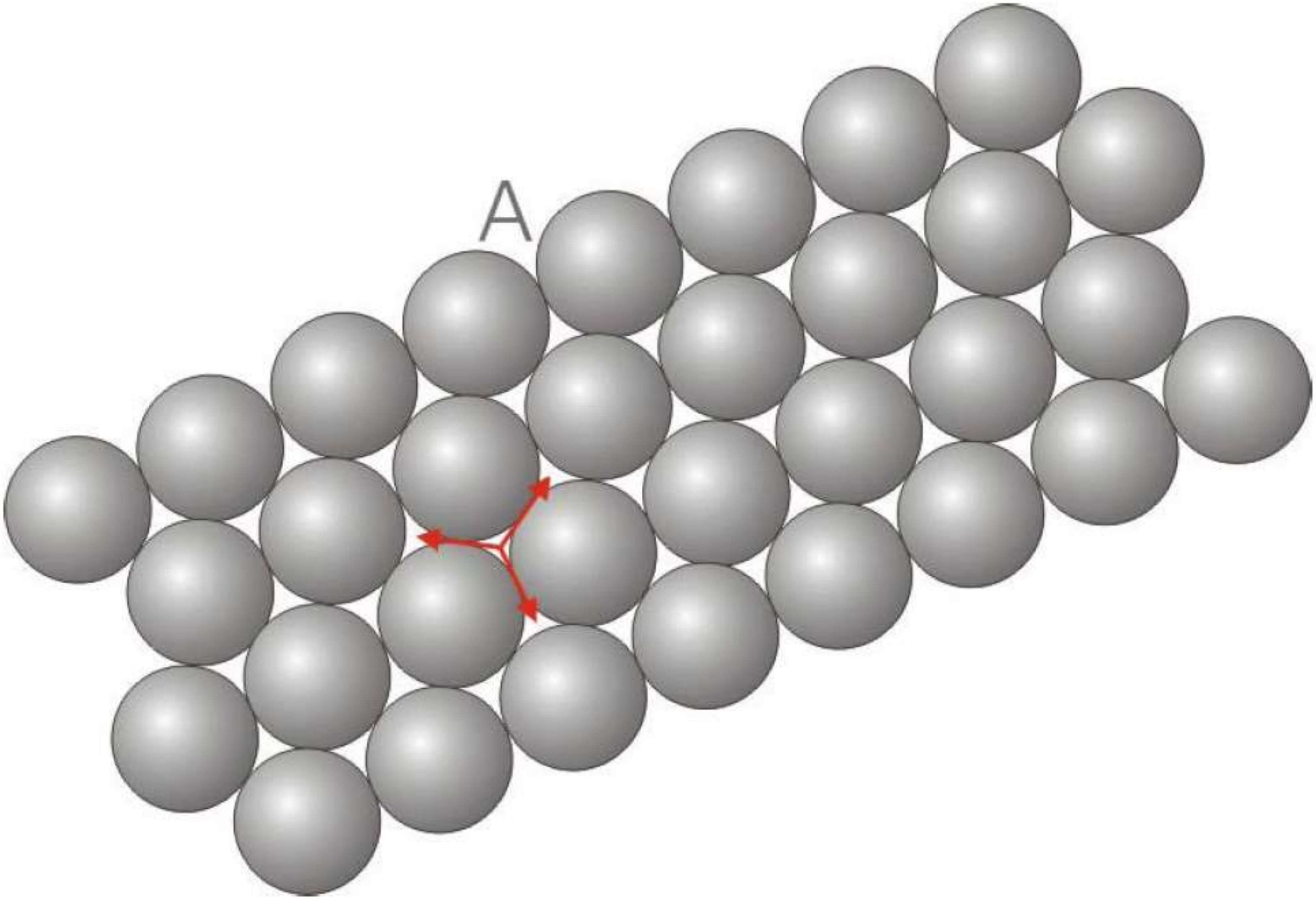


S. Sandlöbes et al. / Acta Materialia 70 (2014) 92–104

Crystal structure: Hexagonal / FCC



Crystal structure: Hexagonal / FCC



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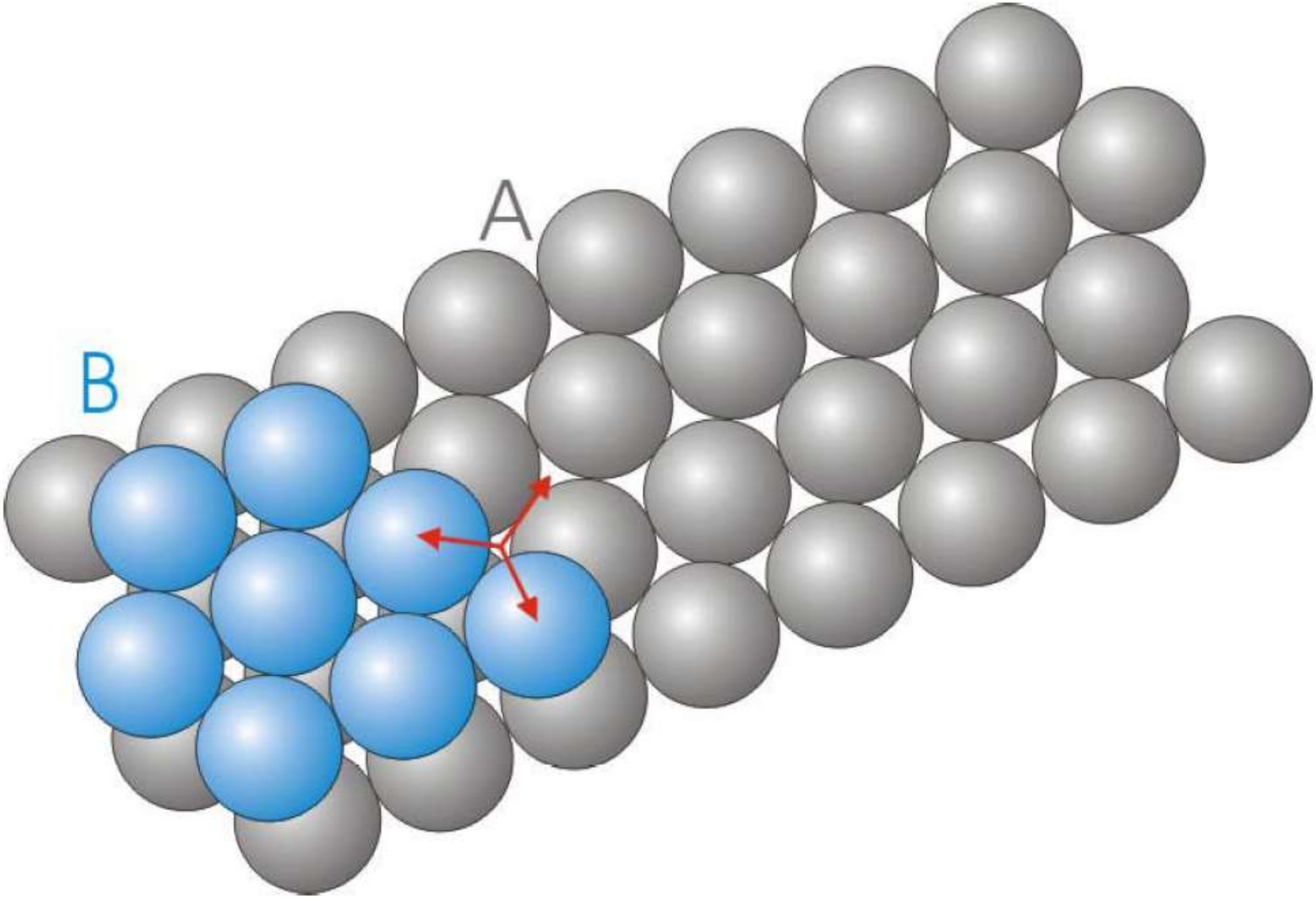

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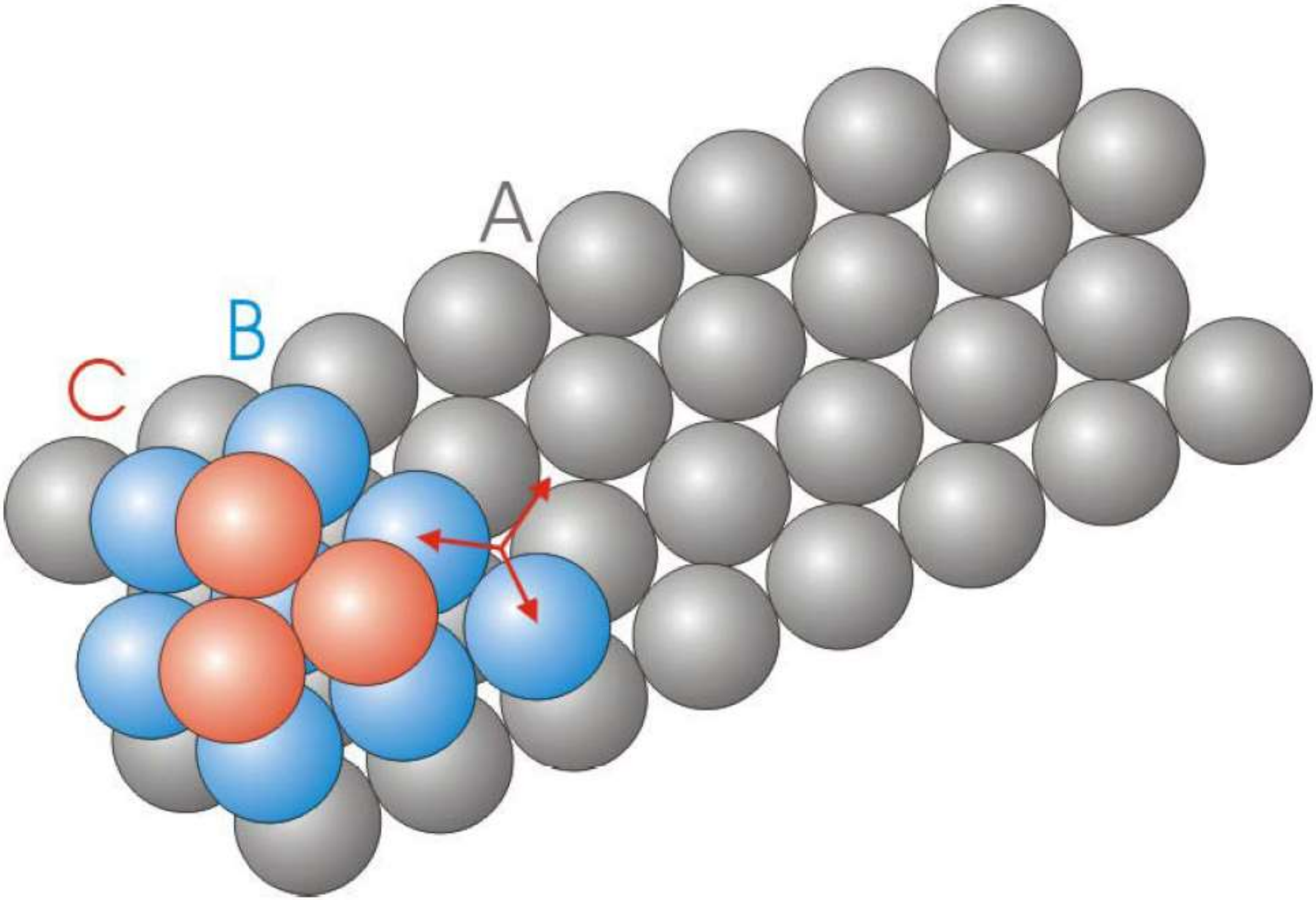
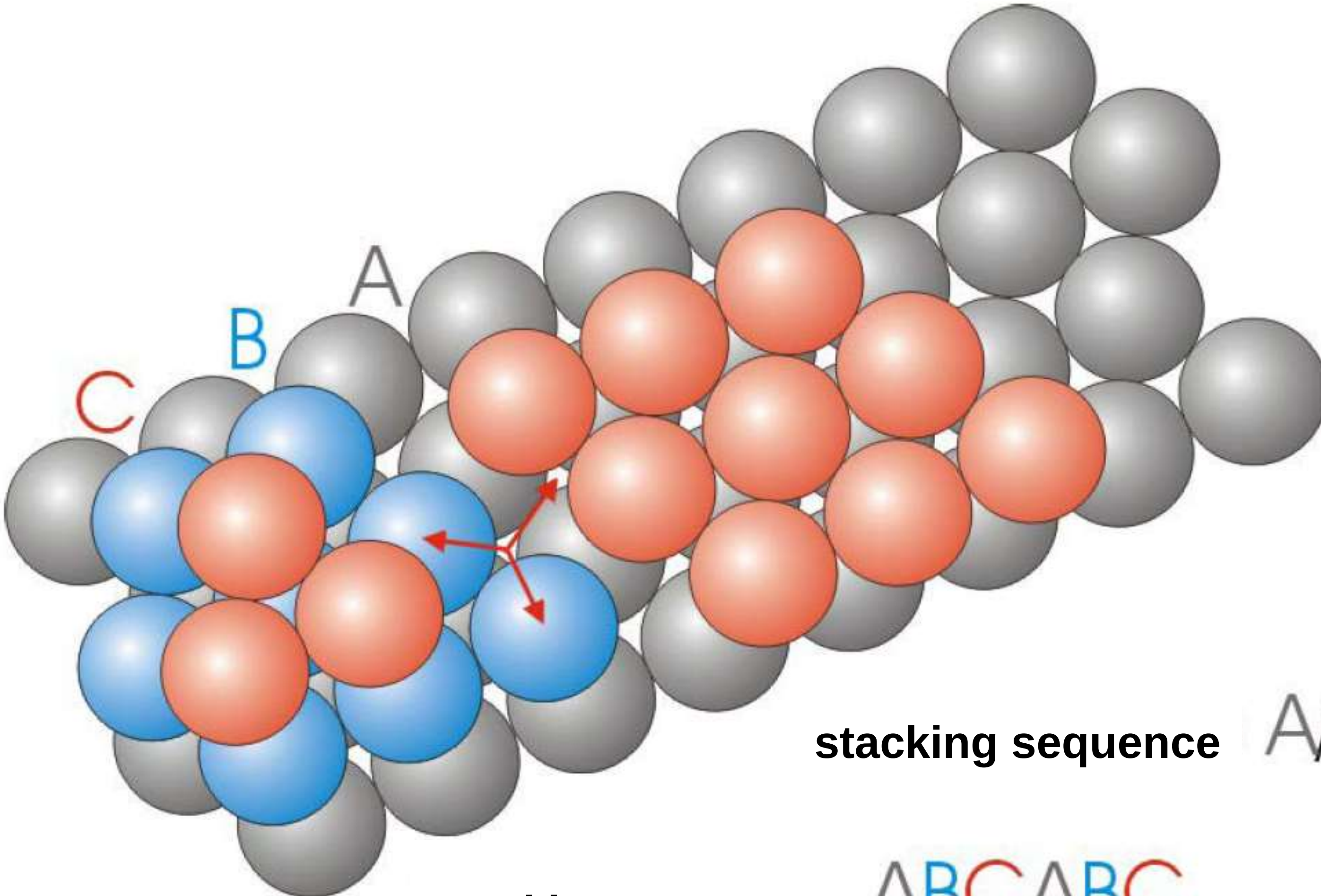


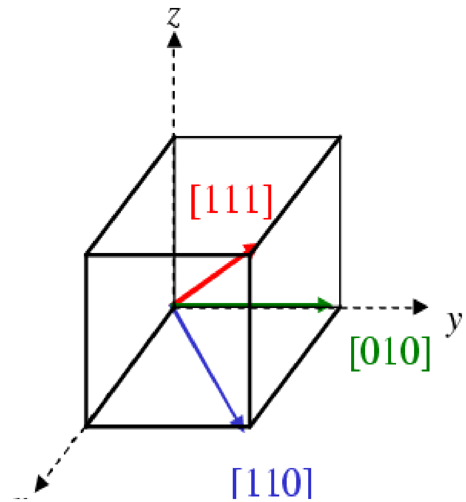
Crystal structure: Hexagonal / FCC

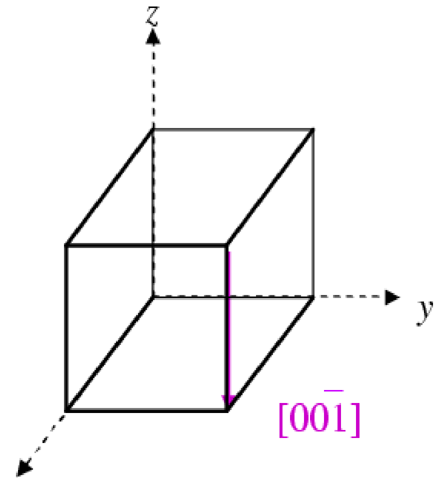


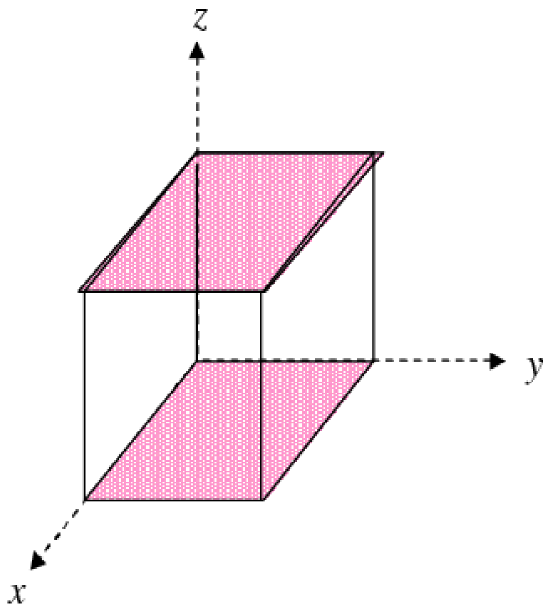
stacking sequence A/CABC

stacking sequence ABCABC

Deriving Miller indices: the description of lattice vectors

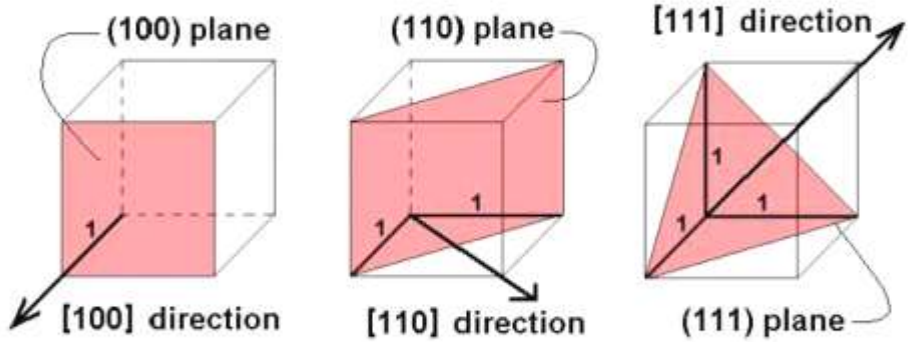


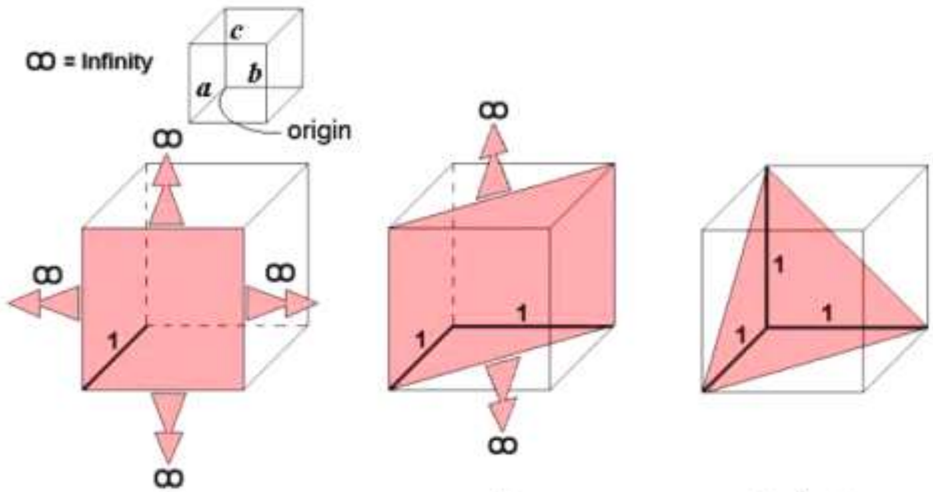




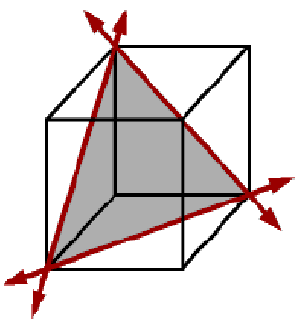
	x	y	z
Intercepts	∞	∞	1
reciprocals	0	0	1
Indices		(001)	

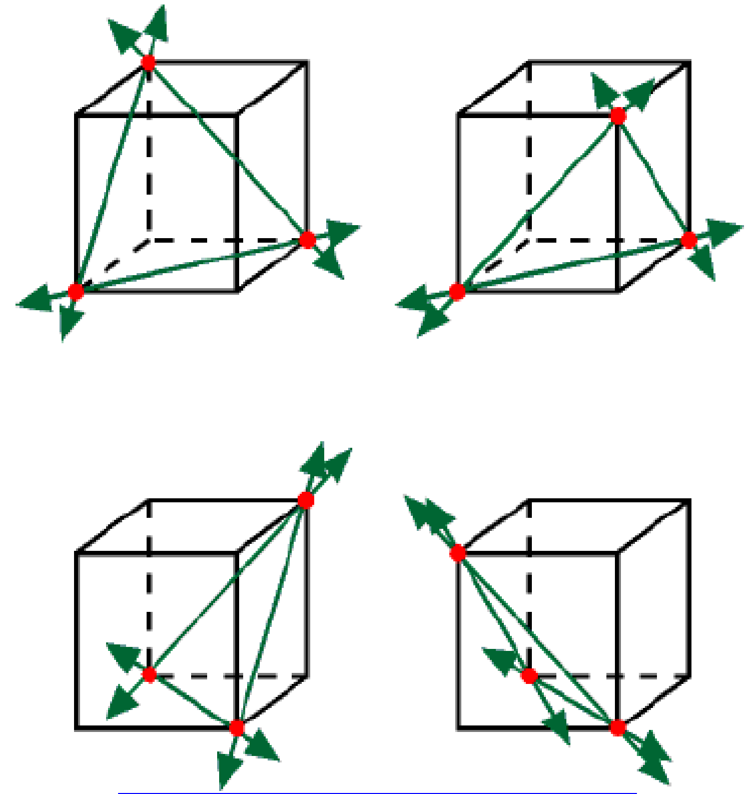
Deriving Miller indices: the description of lattice vectors





$a,\ b,\ c,$	$a,\ b,\ c,$	$a,\ b,\ c,$
$1, \infty, \infty,$	$1,\ 1,\ \infty,$	$1,\ 1,\ 1,$
$\frac{1}{1}\ \frac{1}{\infty}\ \frac{1}{\infty}$	$\frac{1}{1}\ \frac{1}{1}\ \frac{1}{\infty}$	$\frac{1}{1}\ \frac{1}{1}\ \frac{1}{1}$
$=1,\ 0,\ 0,$	$=1,\ 1,\ 0,$	$=1,\ 1,\ 1,$

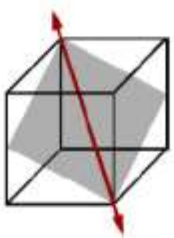
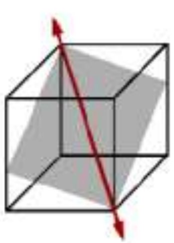
Gitter	Beispiel		Gleitebenen G		Gleitrichtung g		Gesamtzahl der Gleitsysteme
			Typ	Zahl	Typ	Zahl	
kfz	Al Cu Ni Ag Au		(111)	4	[110]	3	12

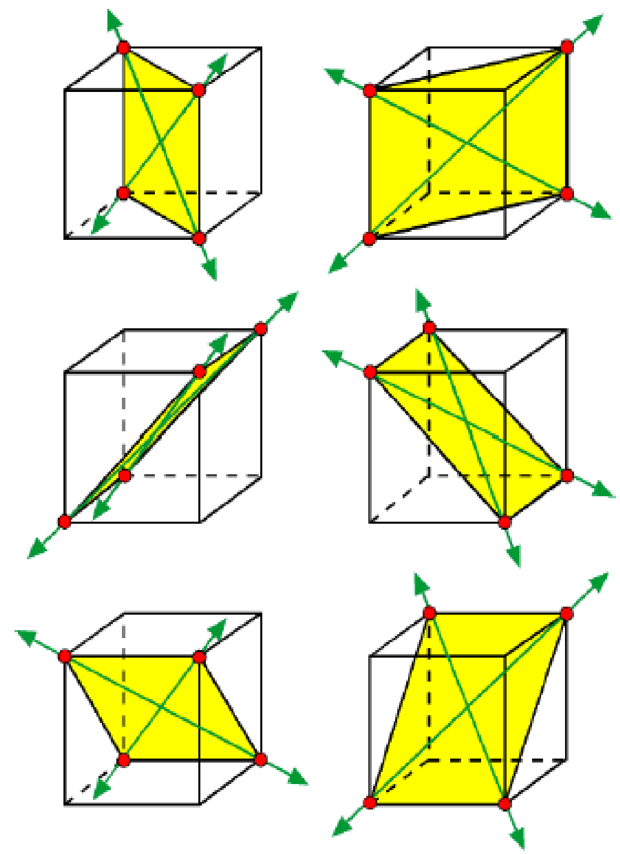


kfz

4E	x	3R	= 12
(111)		[110]	

Miller Indices of typical planes and directions in BCC metals

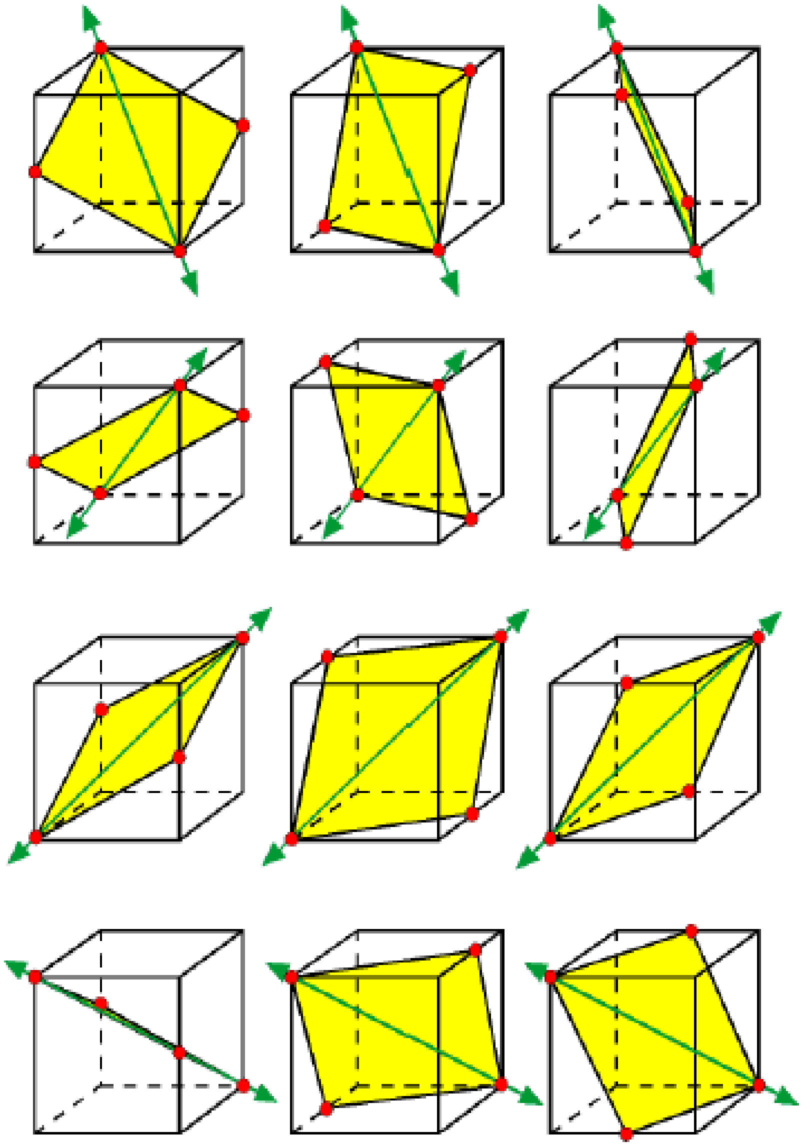
Gitter	Beispiel		Gleitebenen G Typ	Gleitebenen G Zahl	Gleitrichtung g Typ	Gleitrichtung g Zahl	Gesamtzahl der Gleitsysteme
krz	$Fe_{\alpha\delta}$ W Mo Nb Ta		(110)	6	[111]	2	12
	$Fe_{\alpha\delta}$ W Mo Nb		(112)	12	[111]	1	12
	$Fe_{\alpha\delta}$ W_a Mo		(123)	24	[111]	1	24



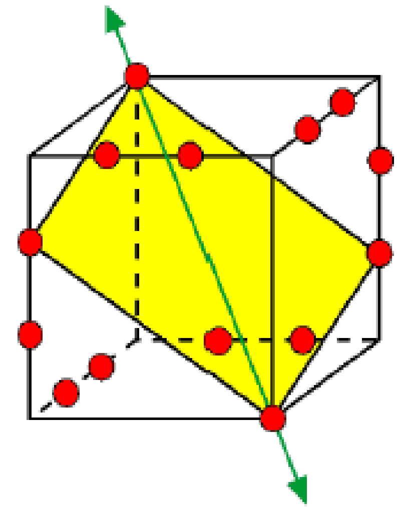
krz

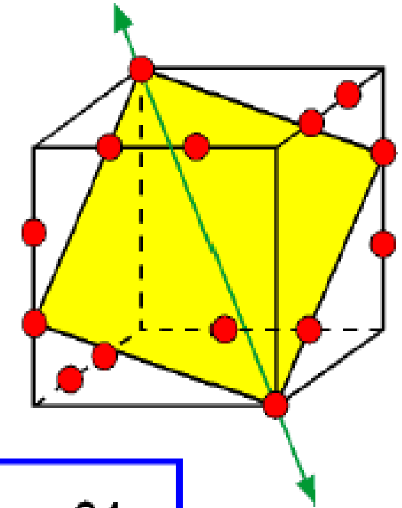
6E	x	2R	= 12
(110)		[111]	

Miller Indices of typical planes and directions in BCC metals



12E x 1R = 12
(112) [111]





24E x 1R = 24
(123) [111]

$$<100> = [1,0,0],[\bar{1},0,0],[0,1,0],[0,\bar{1},0],[0,0,1],[0,0,\bar{1}]$$

$$<110> = [1,1,0],[\bar{1},1,0],[1,\bar{1},0],[\bar{1},\bar{1},0],[1,0,1],[\bar{1},0,\bar{1}],\ldots\ldots$$

	specific	general
direction	[ ]	< >
plane	( )	{ }

vectors and planes

Microstructure Mechanics

Dislocation statics

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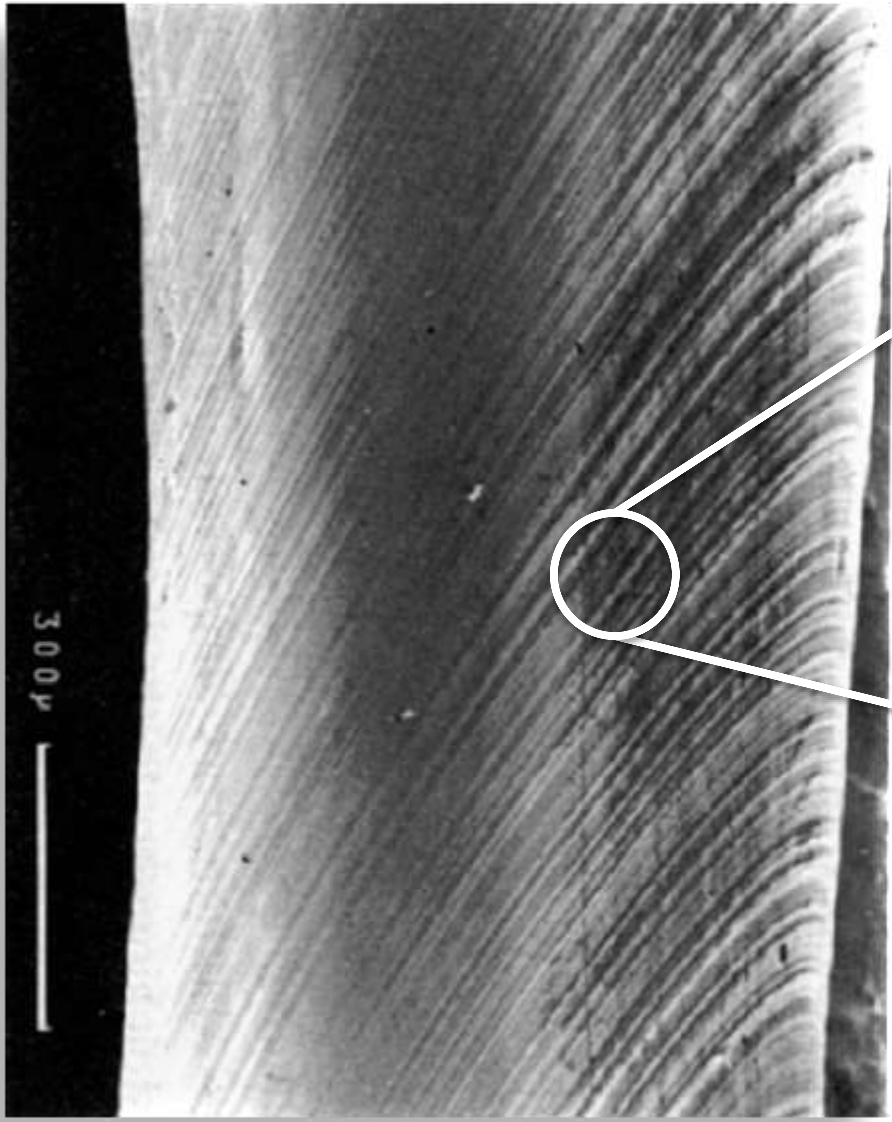
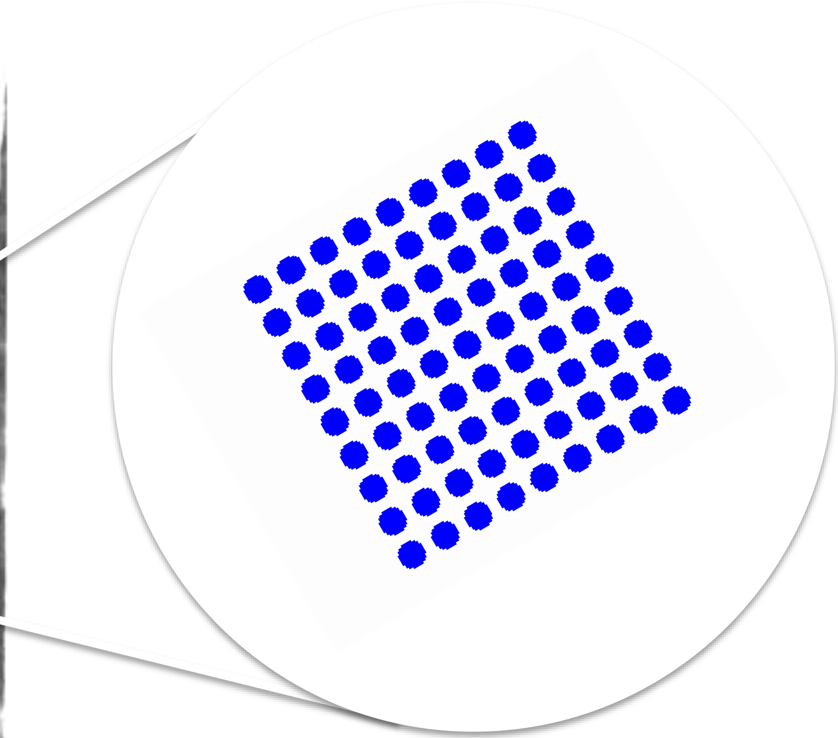
Plastic deformation of a single crystal by dislocation slip

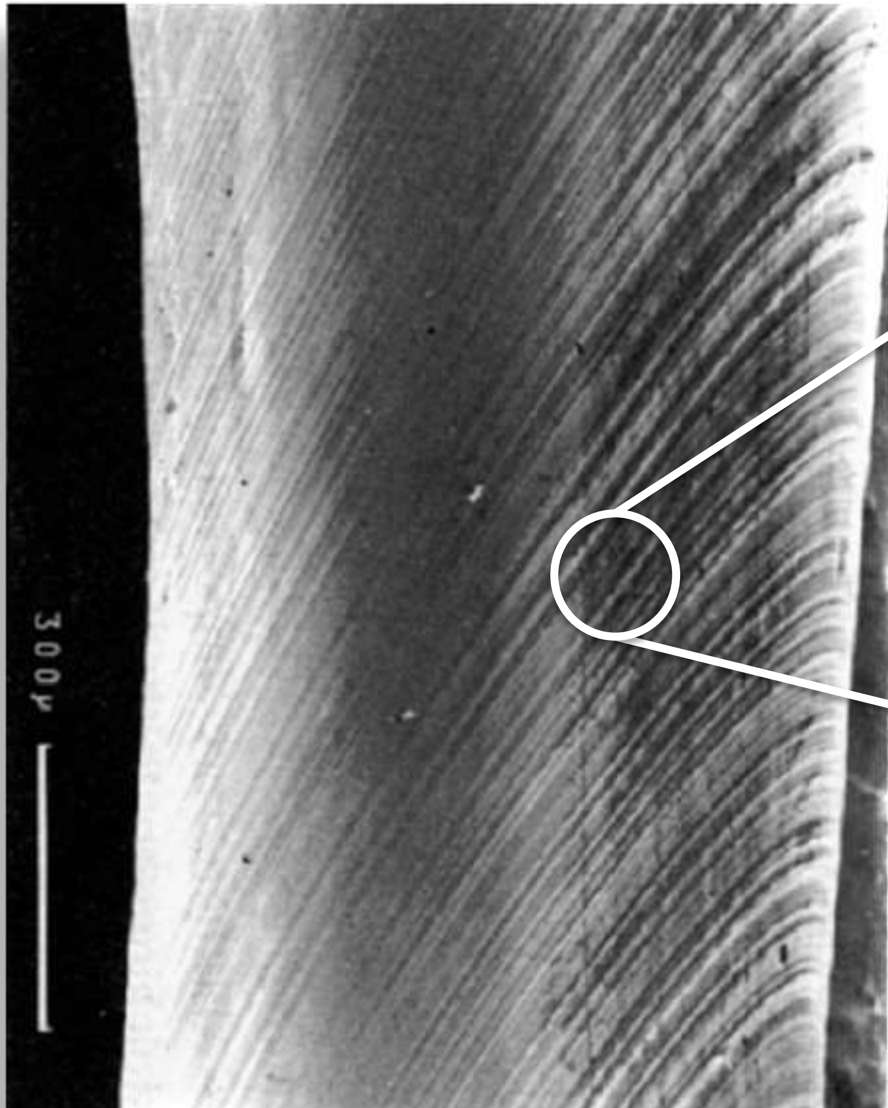


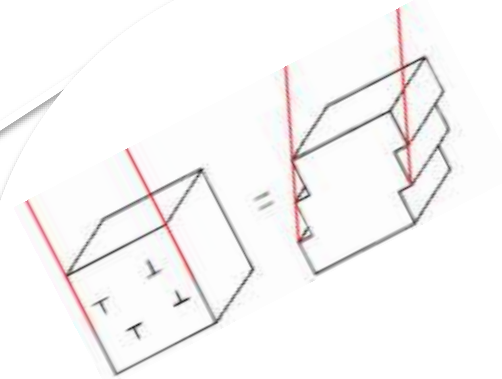
single slip in a single crystal



plastic anisotropy

Plastic deformation of a single crystal by dislocation slip





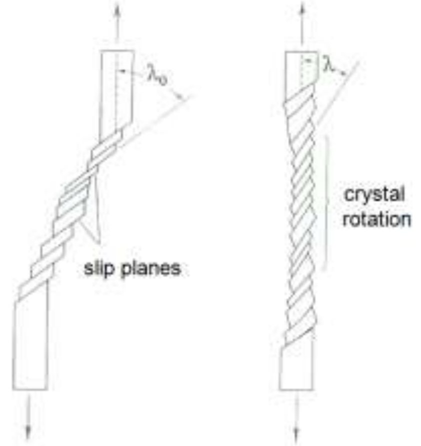
$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

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:

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

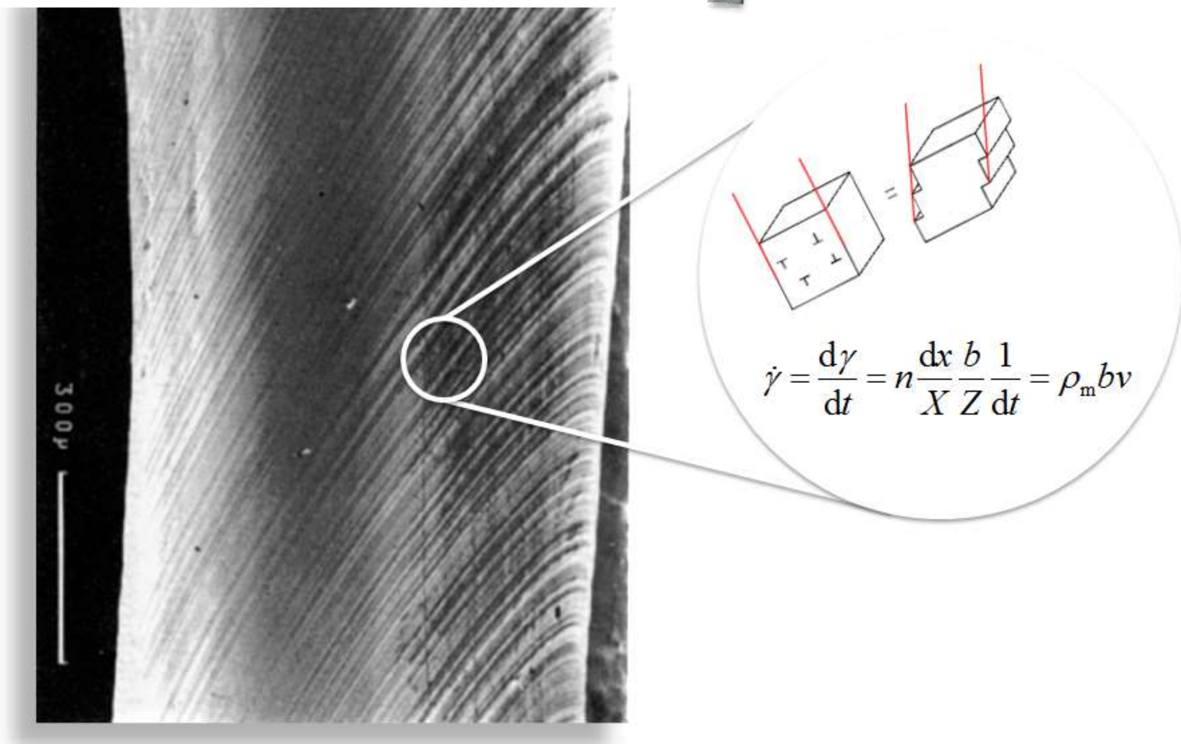
$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)_{etc.}$$

Strain tensor: symmetrical part of displacement gradient tensor

Roters et al. Acta Mater.58 (2010)

strain rates and displacement gradients in crystals

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

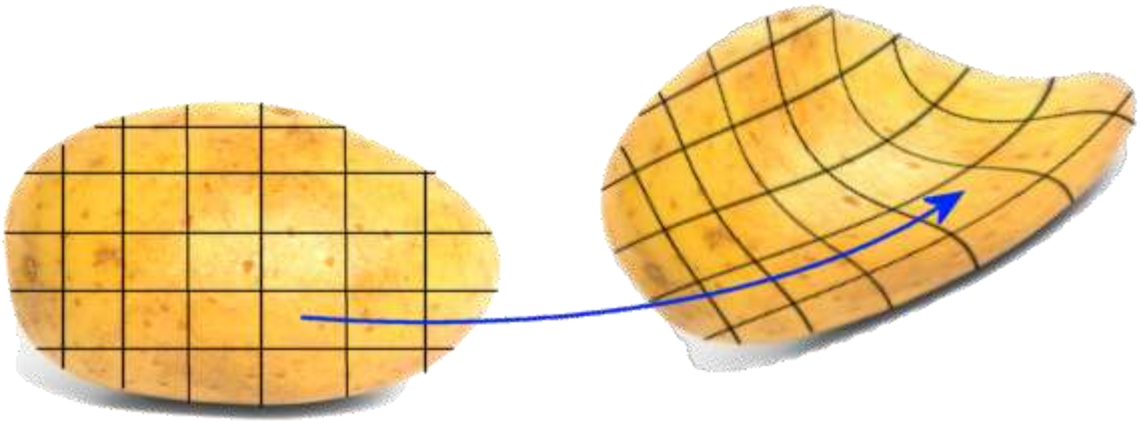


strain rates and displacement gradients in crystals

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

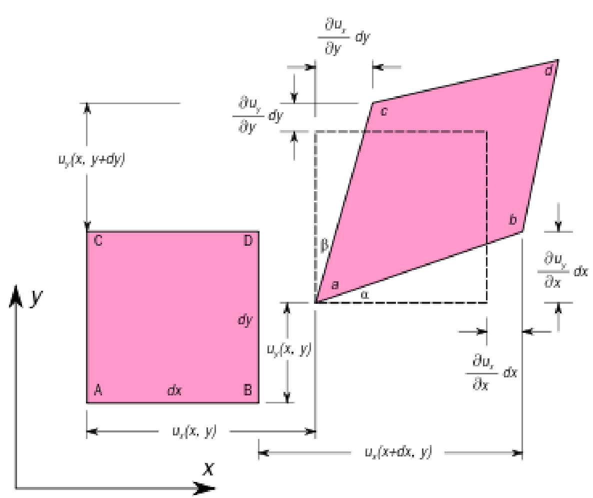
plastic spin from polar decomposition

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



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

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



Roters et al. Acta Mater.58 (2010)

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

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

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

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

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

$$= \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) & \frac{1}{2}\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right) \\ \frac{1}{2}\left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2}\right) & \frac{\partial u_2}{\partial x_2} & \frac{1}{2}\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right) \\ \frac{1}{2}\left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3}\right) & \frac{1}{2}\left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3}\right) & \frac{\partial u_3}{\partial x_3} \end{bmatrix}$$

Displacement gradient tensor: the rotation

Rotation tensor

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

In matrix form

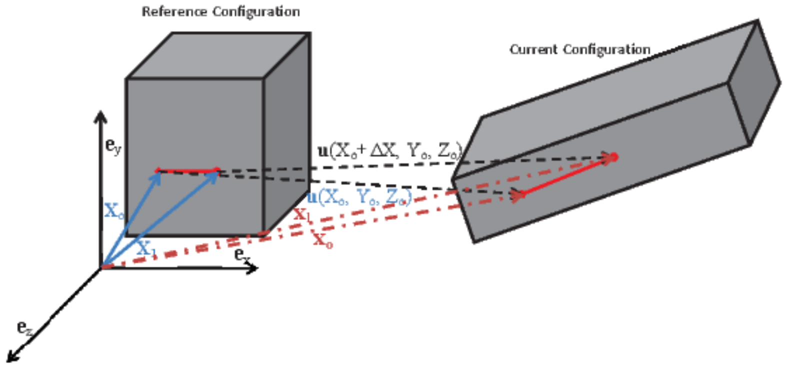
$$\omega = \frac{1}{2}\left(\nabla \mathbf{u} - (\nabla \mathbf{u})^T\right)$$

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

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

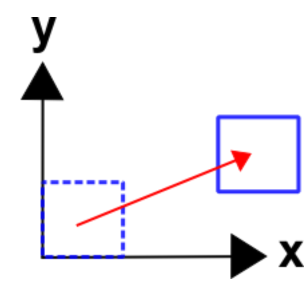
Shear strains

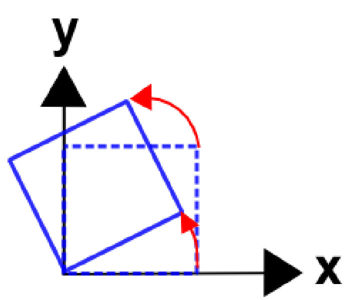
$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$
$$\varepsilon_{xz} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)$$
$$\varepsilon_{yz} = \frac{1}{2}\left(\frac{\partial v}{\partial z} + \frac{\partial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

Engineering shear strains

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

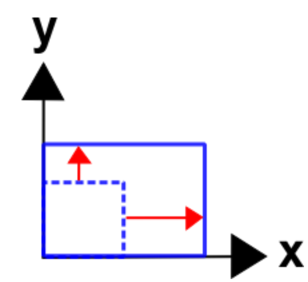
Rigid Body Displacements

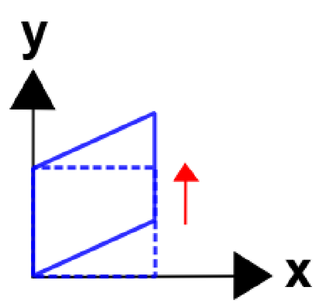




Rigid Body Rotations

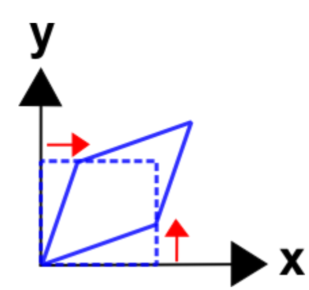
Stretching

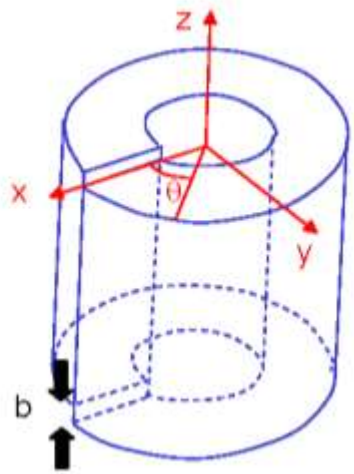




Shear (with Rotation)

Pure Shear





"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

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

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

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

$$\Downarrow$$

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

$$\Delta = 0$$

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

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

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

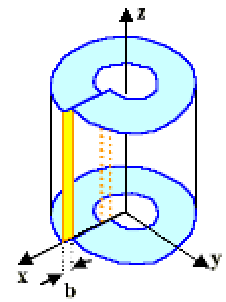
$$\underline{u}(\underline{x}) = \begin{pmatrix} 0 \\ 0 \\ \frac{b}{2\pi} \arctan \frac{y}{x} \end{pmatrix}$$

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

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

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

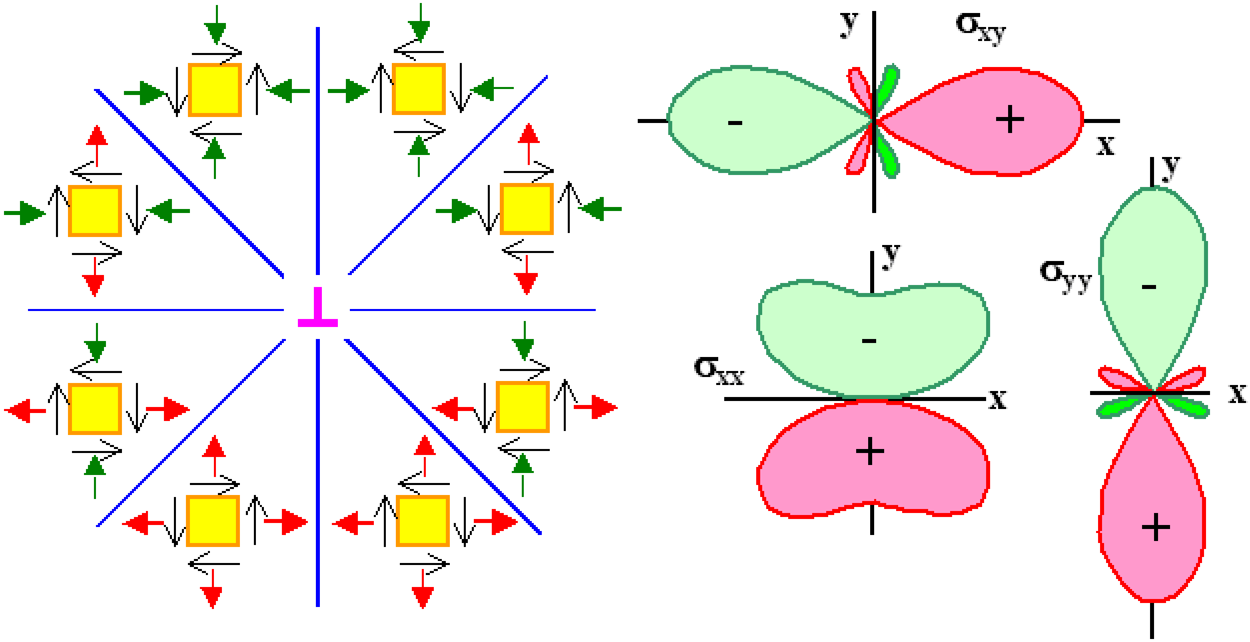
$$\sigma_{xx} = \frac{b\,G\,y\,\left(3\,x^2 + y^2\right)}{2\,\left(-1+\nu\right)\,\pi\,\left(x^2+y^2\right)^2}$$

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

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

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

Forces and stress field: infinite straight edge dislocation



Microstructure Mechanics

Dislocation dynamics

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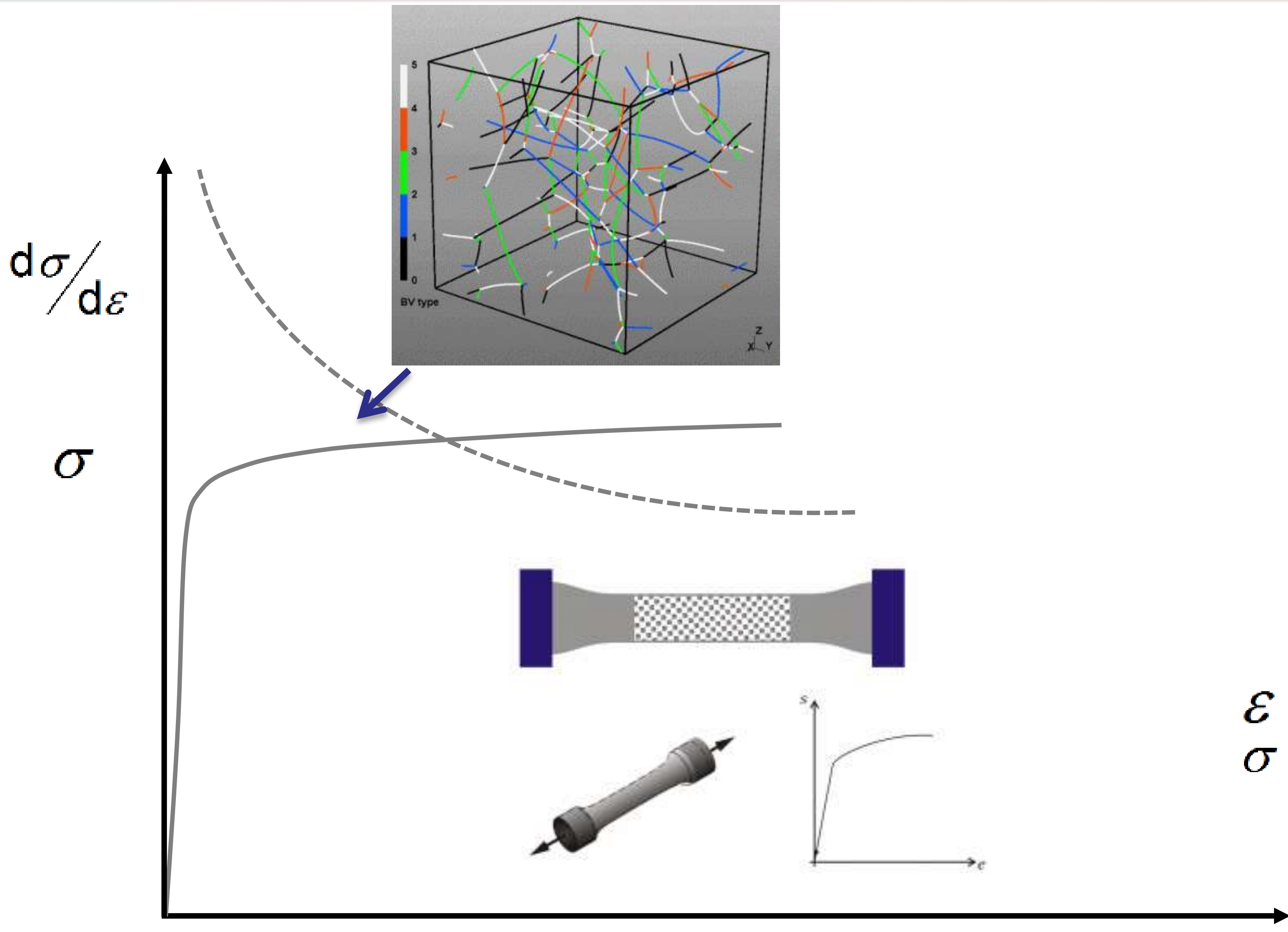
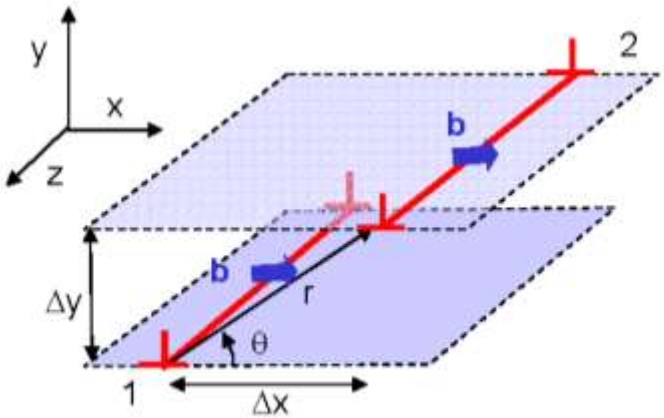


ε

ε true strain

σ stress

Dynamics: forces among dislocations



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

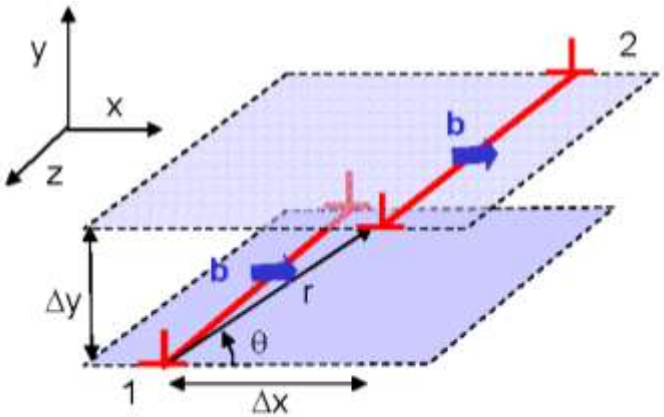
Peach-Koehler Force

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

$\boldsymbol{\sigma_{xy}}$ – produces *glide* force

$\boldsymbol{\sigma_{xx}}$ – produces *climb* force

Forces among edge dislocations

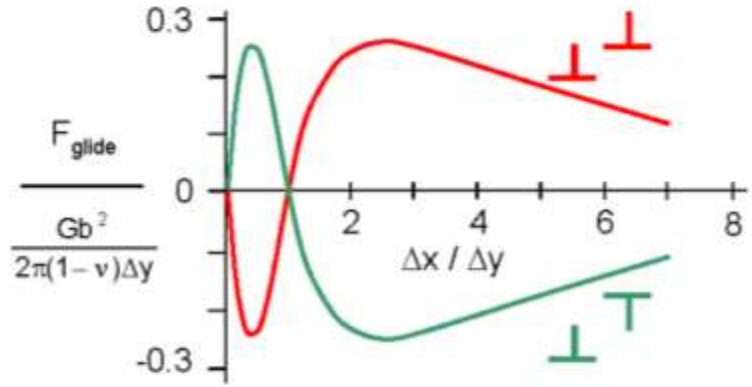


$$\sigma_{xx} = -D y \frac{3\Delta x^2 + \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}, \quad \text{with: } D = \frac{Gb}{2\pi(1-\nu)}$$

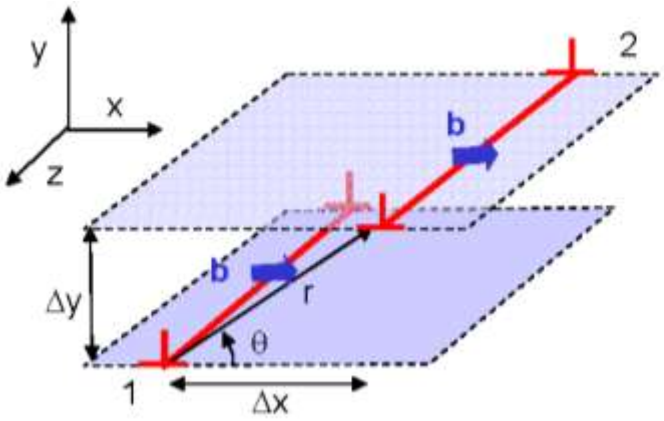
$$\sigma_{xy} = \sigma_{yx} = D\,\Delta x \frac{\Delta x^2 - \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}$$

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

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

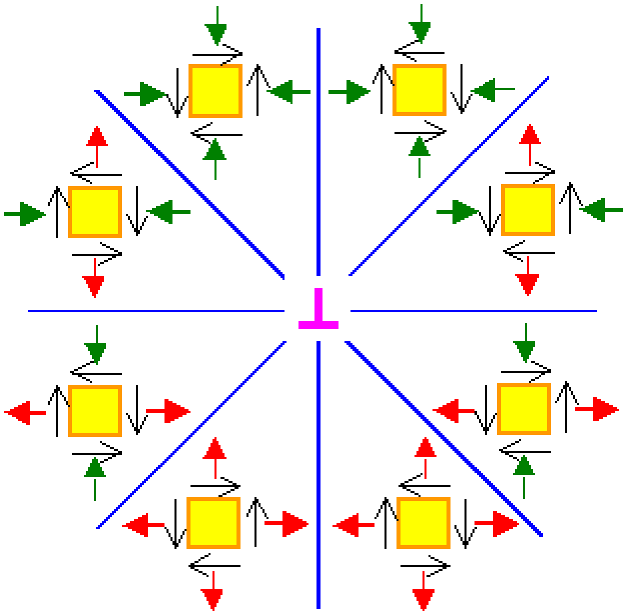


Forces among edge dislocations

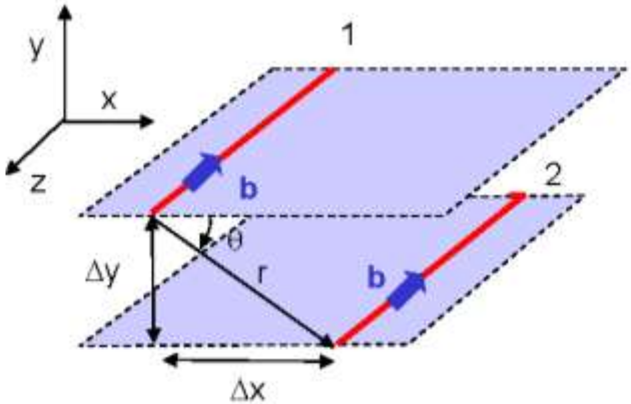


$$\sigma_{xx} = -D\,y\,\frac{3\Delta x^2 + \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}, \quad \text{with: } D = \frac{Gb}{2\pi(1-\nu)}$$

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



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:

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

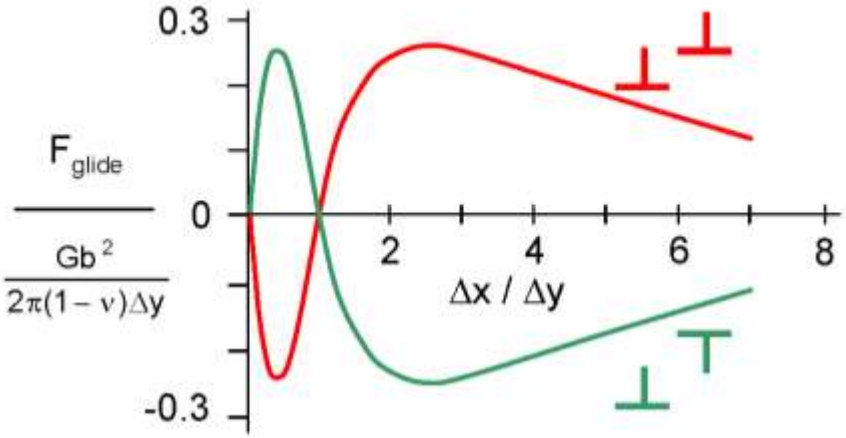
$$\sigma_{xz} = -\frac{Gb}{2\pi}\frac{\Delta y}{\Delta x^2 + \Delta y^2} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

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

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



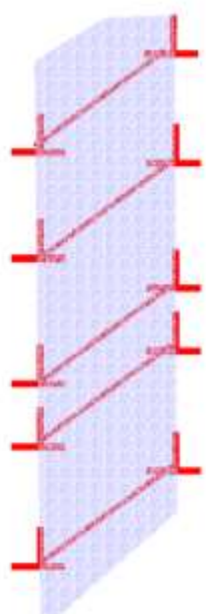
For **like** Burgers vectors:
$\Delta x = \pm\Delta y$: unstable equilibrium
$\Delta x = 0$: stable equilibrium

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

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

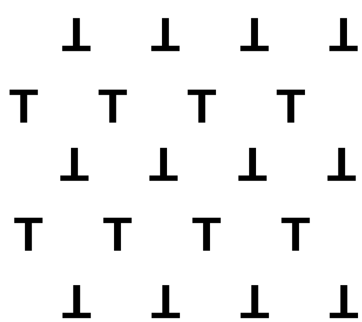
A low angle tilt boundary.

This arrangement has a strong long-range stress field.

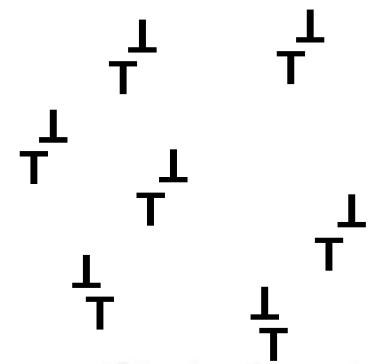


For a set of **"opposite"** Burgers vectors:

There are a large number of possible stable



"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)

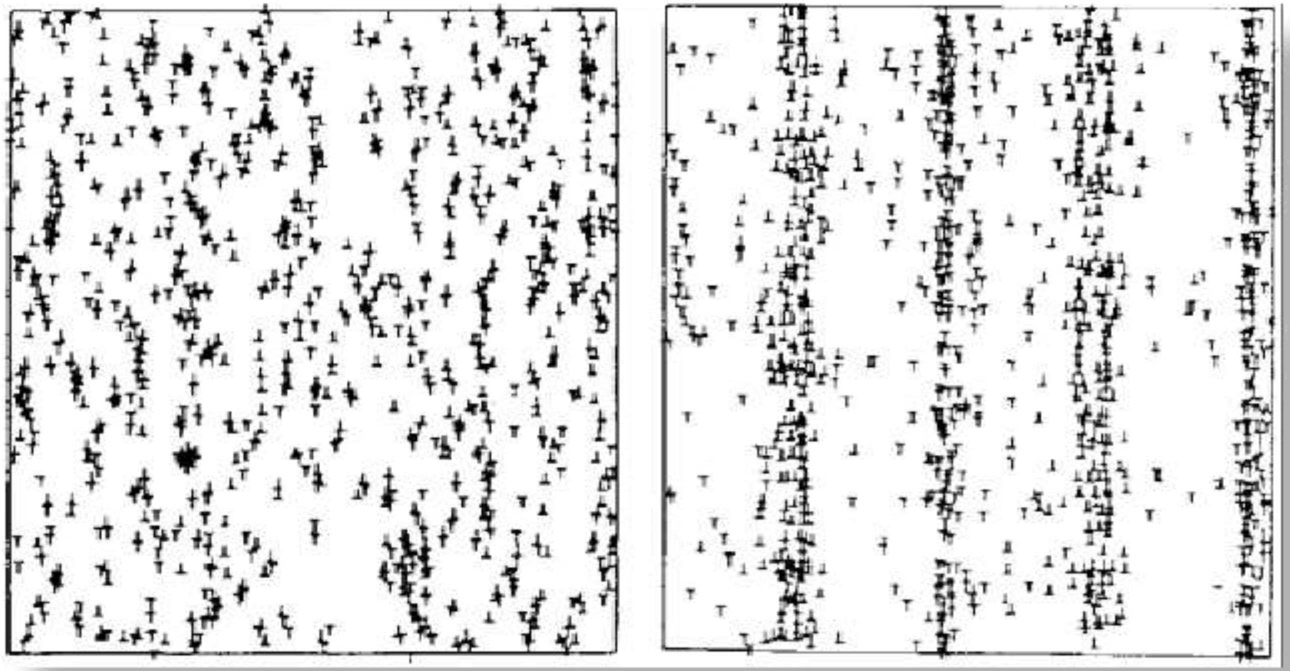
Discrete Dislocation Dynamics

Statistical Dislocation Dynamics

Discrete Dislocation Dynamics

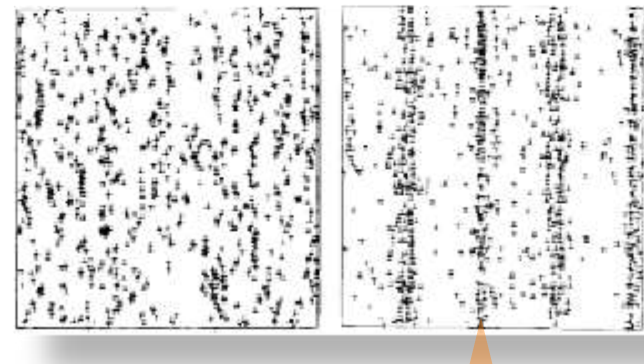
Discrete Dislocation Dynamics in 2D

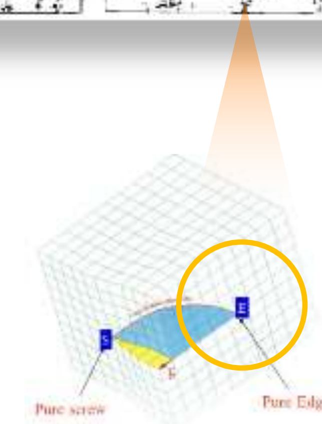
2D – view parallel to dislocation line



Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line





Some questions:

Difference between edge and screw dislocations?

How to do multiplication?

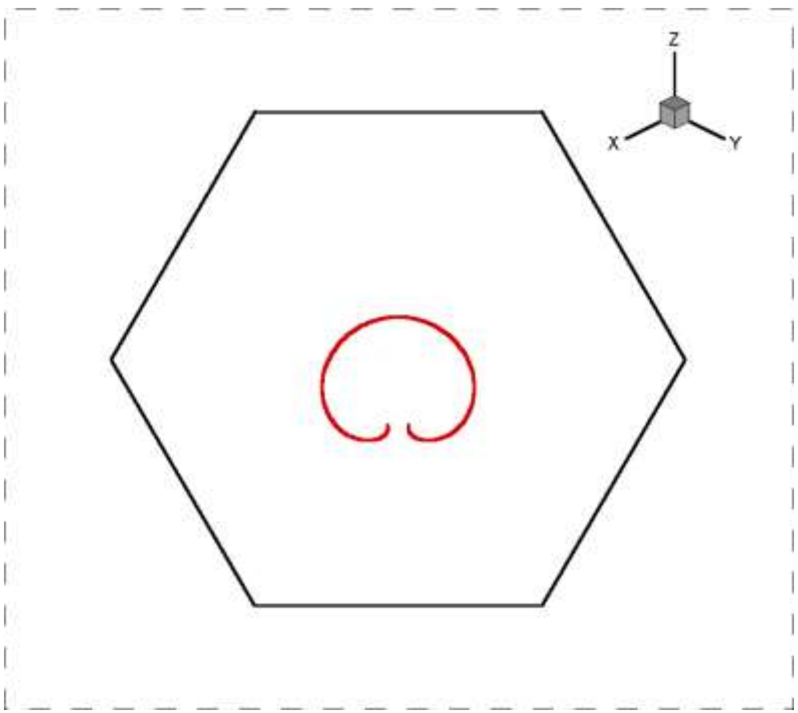
Dislocation bow-out?

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>

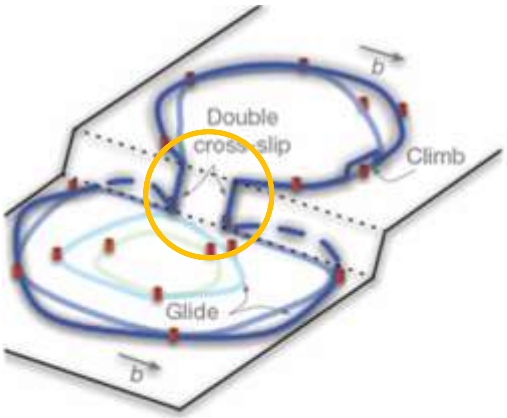
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

Jog-drag?



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

<u>Some questions:</u>

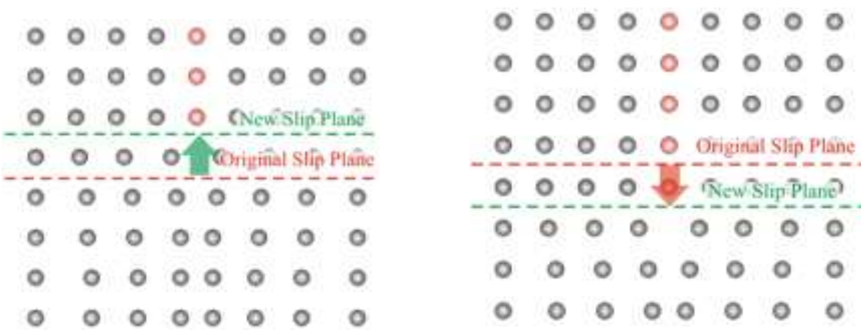
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

Jog-drag?



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

<u>Some questions:</u>

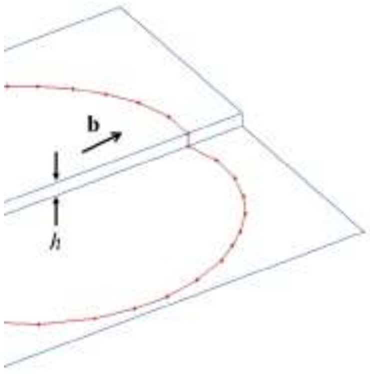
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

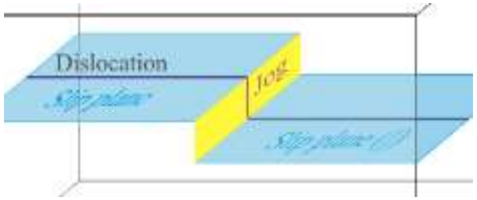
Jog-drag?



Dislocation-Dislocation Interactions

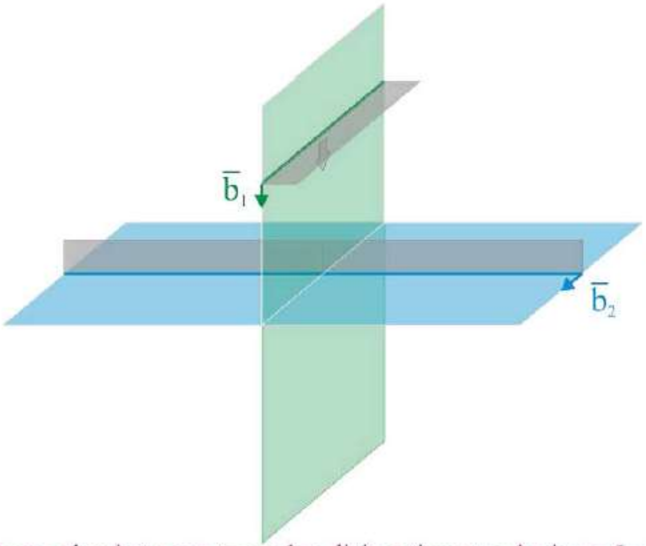
Straight dislocation can intersect to leave Jogs and Kinks in the dislocation line

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

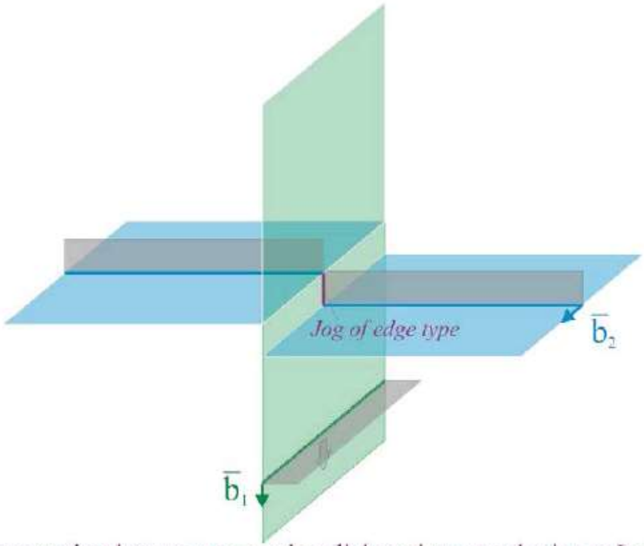


Edge-Edge Intersection Perpendicular Burgers vector

- The jog has edge character and can glide *(with Burgers vector = $\mathbf{b}_2$)*
- 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 $|\mathbf{b}_1|$.

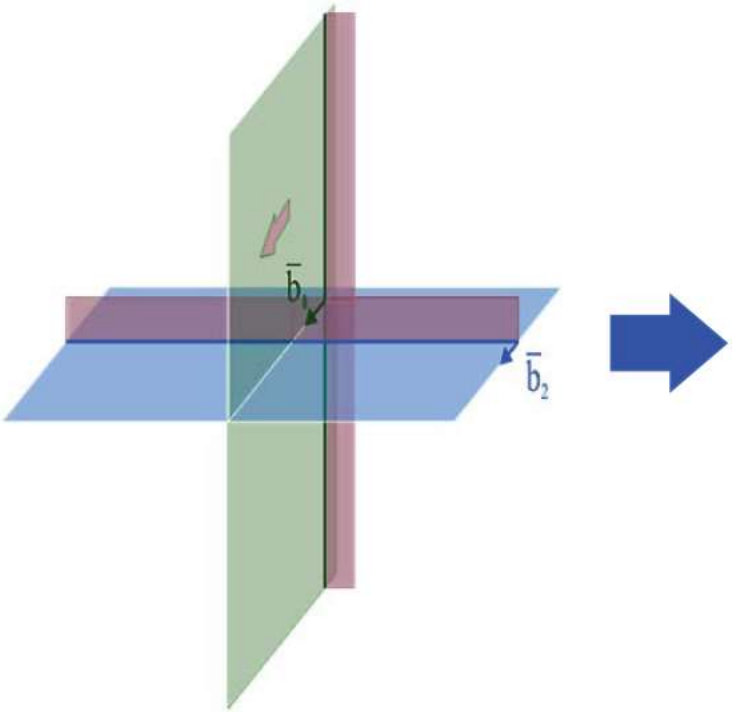


Intersection between two edge dislocations producing a Jog

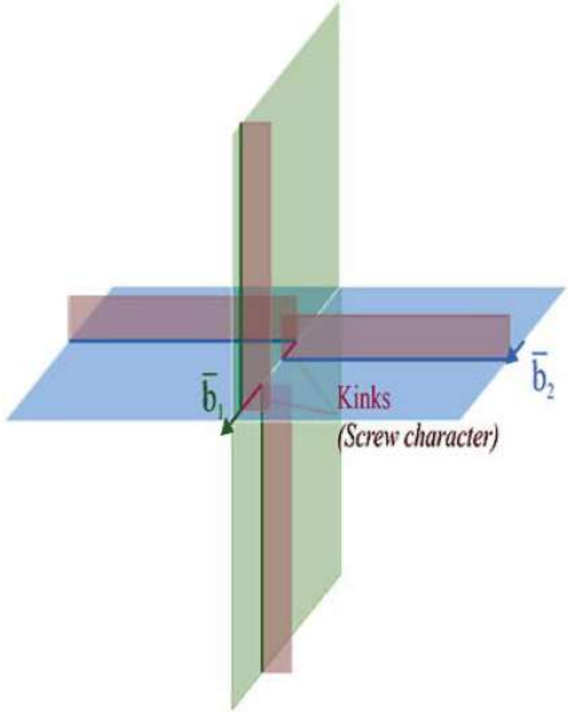


Intersection between two edge dislocations producing a Jog

- 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



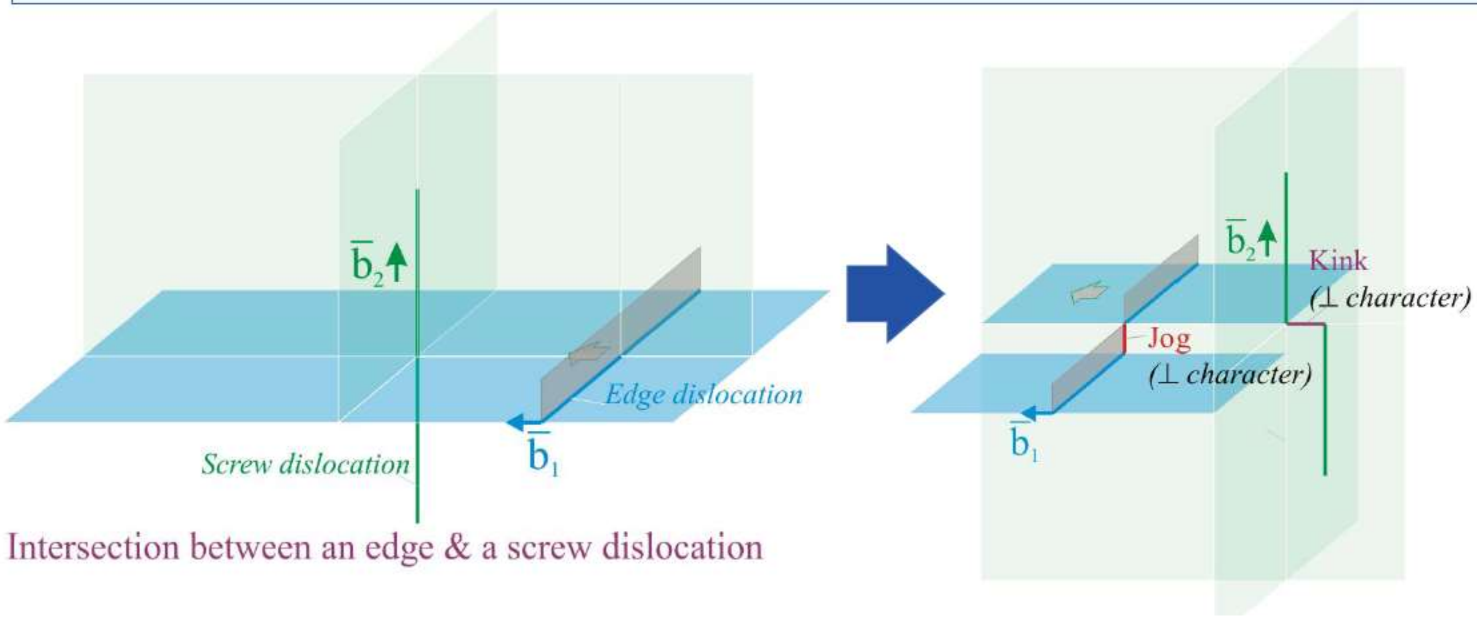
Intersection between two edge dislocations



Intersection between two edge dislocations

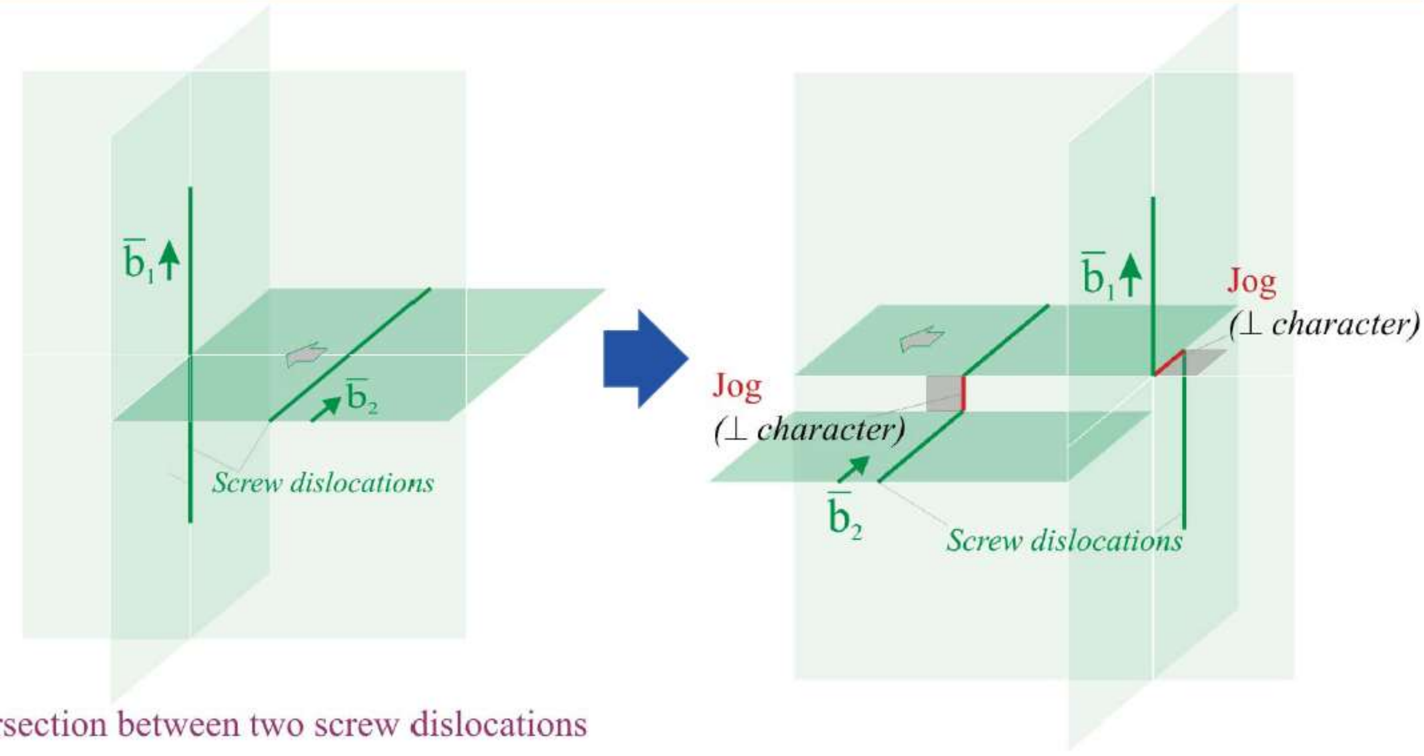
Edge-Screw Intersection Perpendicular Burgers vector

- Edge Dislocation *(Burgers vector* $\mathbf{b}_1$*)* → Jog (Edge Character) → Length $|\mathbf{b}_2|$
- Screw Dislocation *(Burgers vector* $\mathbf{b}_2$*)* → Kink (Edge Character) → Length $|\mathbf{b}_1|$



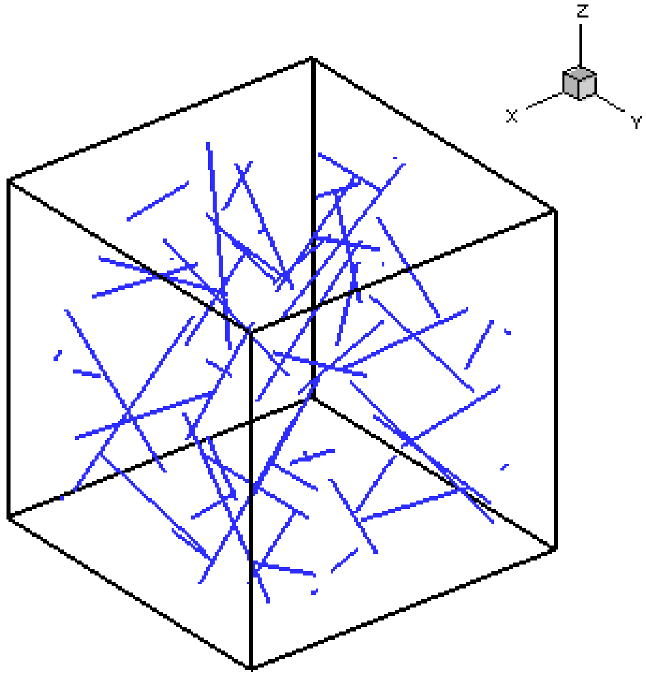
Intersection between an edge & a screw dislocation

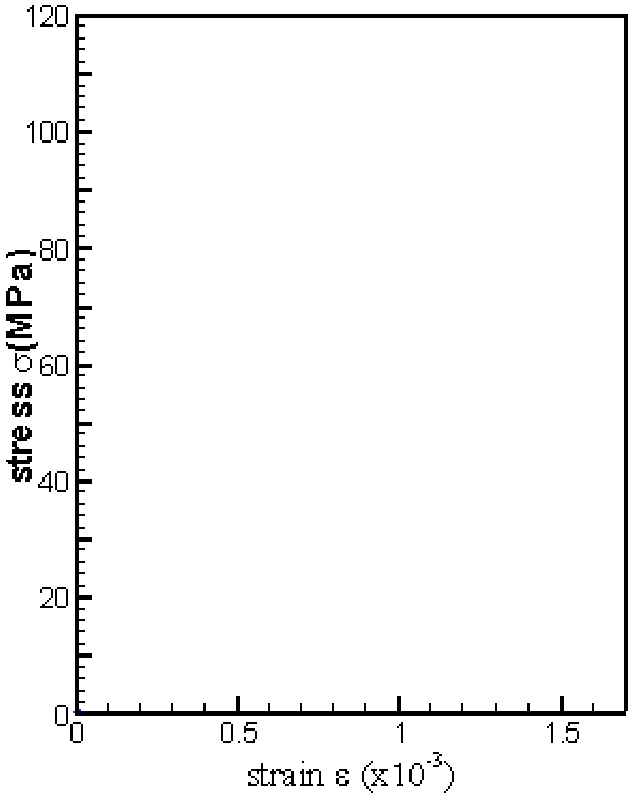
- Important from plastic deformation point of view
- Screw Dislocation *(Burgers vector* $\mathbf{b}_1$*)* → Jog (Edge Character) → Length $\mathbf{b}_2$
- Screw Dislocation *(Burgers vector* $\mathbf{b}_2$*)* → Jog (Edge Character) → Length $\mathbf{b}_1$
- Both the jogs are non conservative
  (i.e. cannot move with the dislocations by glide)



Intersection between two screw dislocations

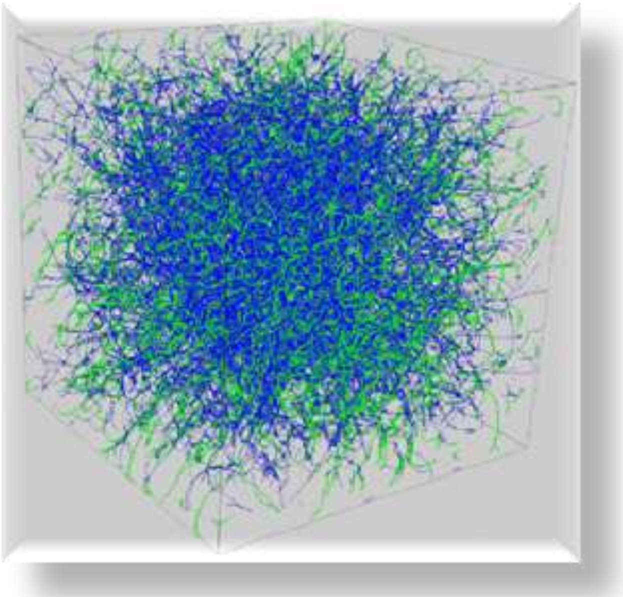
3D: DDD (discrete dislocation dynamics)





Discrete Dislocation Dynamics in 3D

Full 3D segment treatment



Some questions:

Difference between edge and screw dislocations?

Junctions?

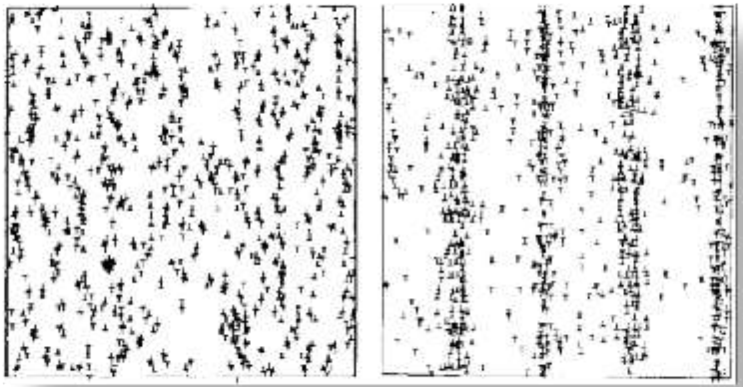
Cutting?

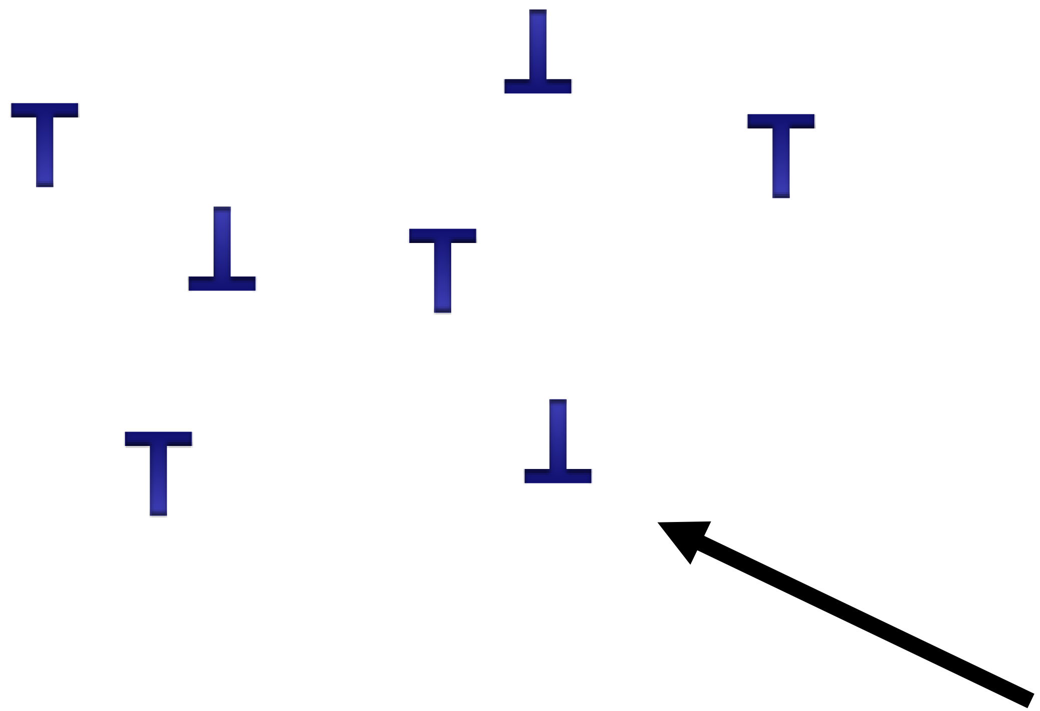
Cores of the dislocations?

Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line

Principle procedure





?

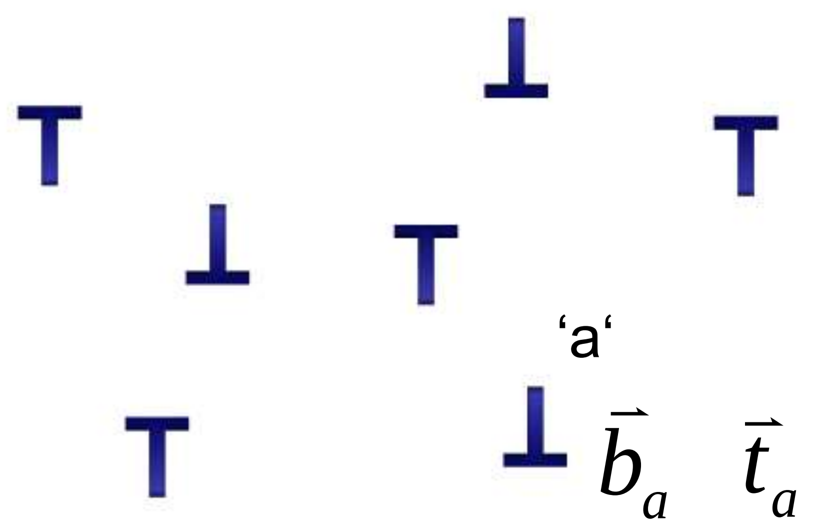
How to proceed?

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

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

Force on dislocation ‘a‘

by all others



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

acceleration

friction coefficient (drag)

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

inertia

velocity

Equilibrium of forces

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

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

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

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

1

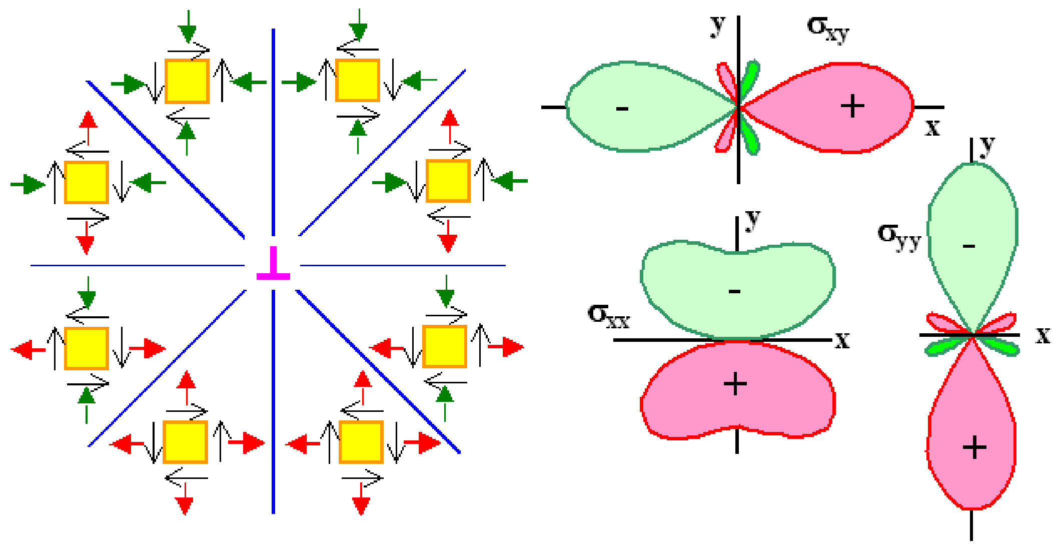
$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0$$

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

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

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

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



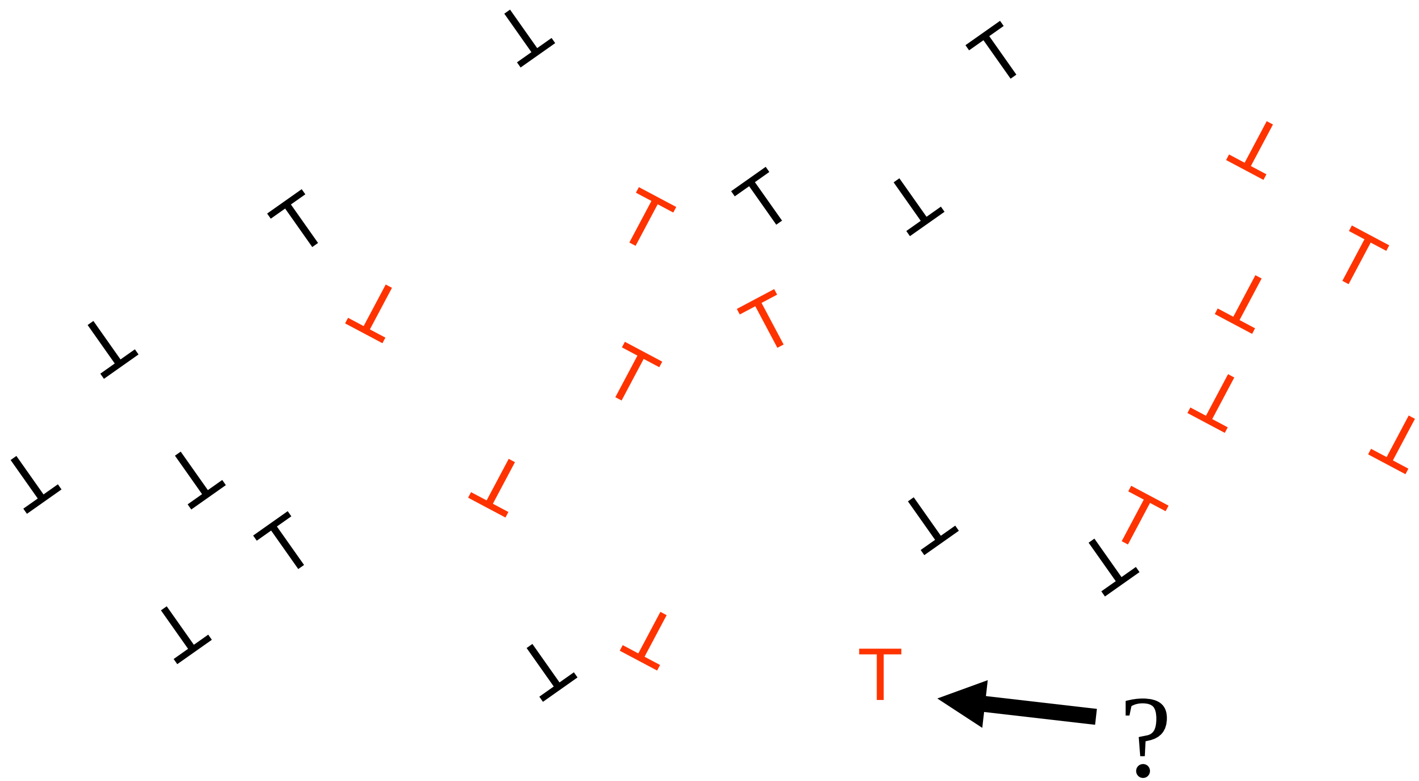
2

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

3

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

Example of Discrete Dislocation Dynamics in 2D



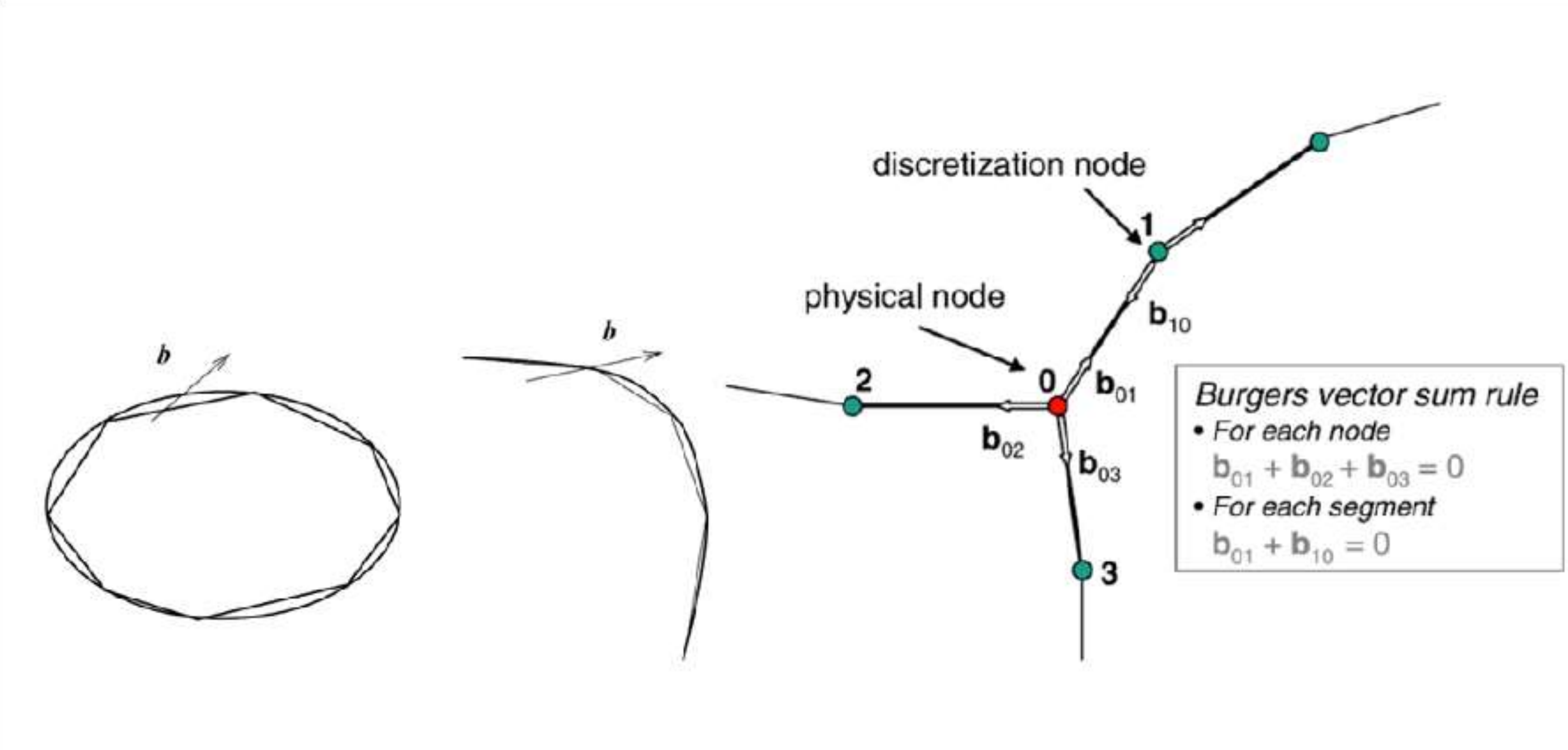
T ← ?

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

3D segments and node construction



Annihilation events

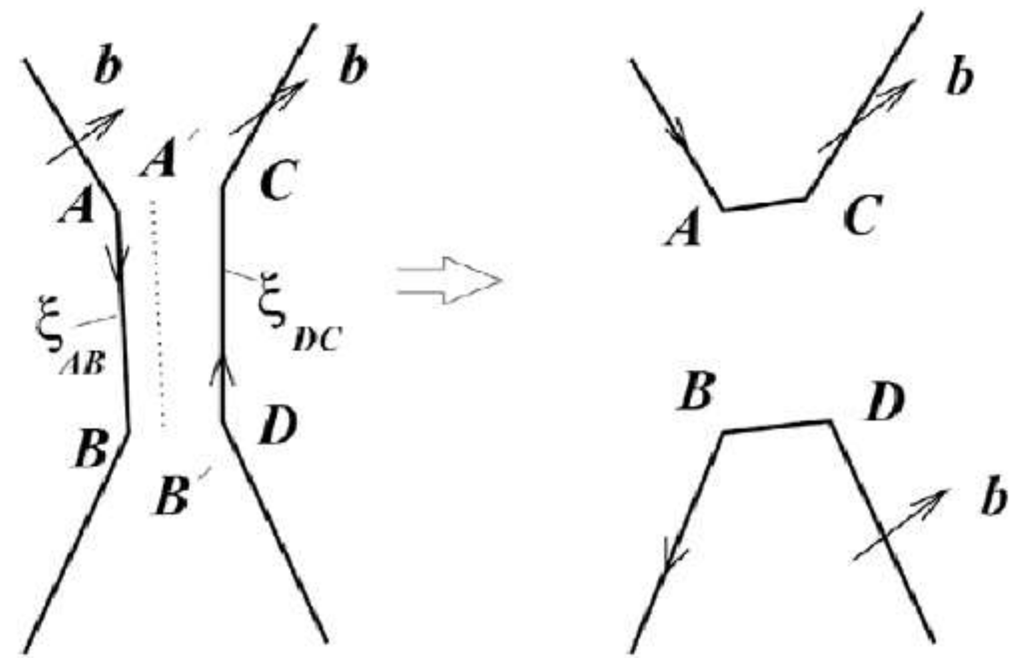


Figure: Annihilation of two attractive dislocations

Jog formation

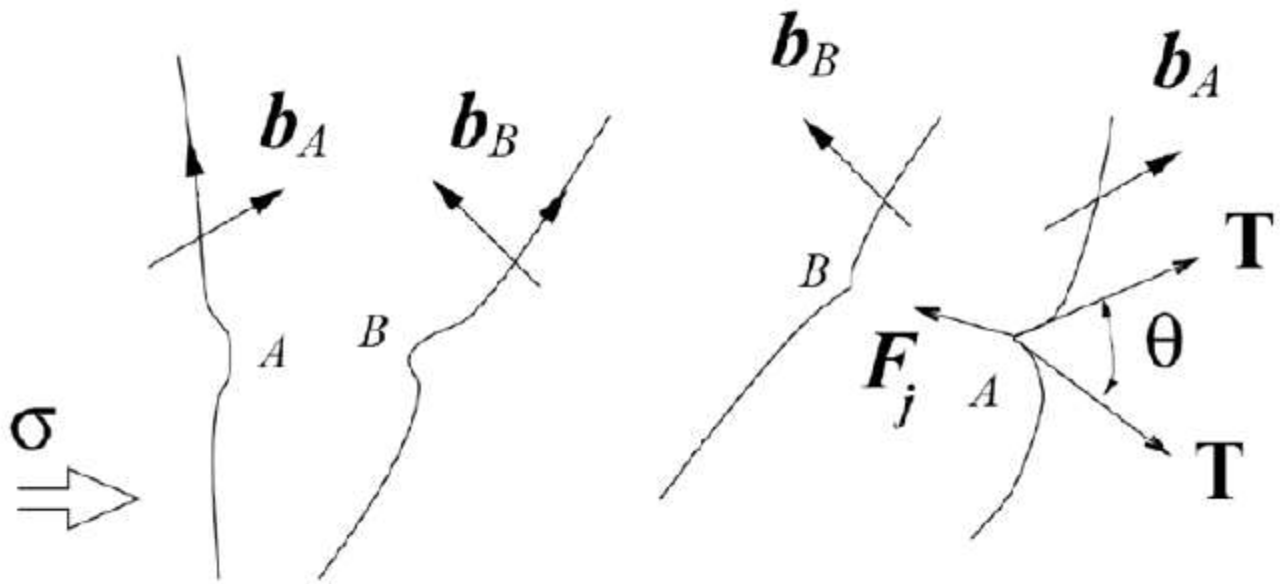


Figure: Jogs are formed when the angle between two attractive dislocations in different planes becomes less than a critical angle θ_c^{jog}

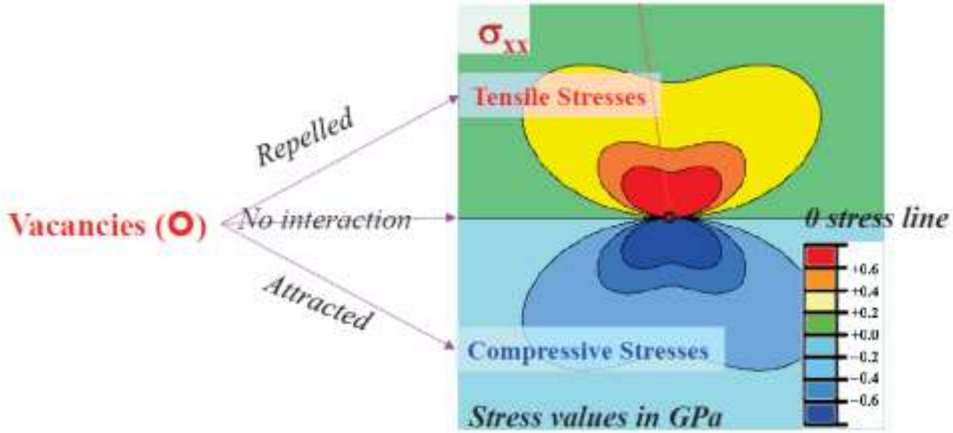
Dislocation-Point Defect Interactions

- The stress field of a dislocation can interact with the stress field of point defects.
- Defects associated with tensile stress fields are attracted towards the compressive region of the stress field of an edge dislocation (*and vice versa). Higher free-volume at the core of the edge* dislocation aids this segregation process.
- Solute atoms can segregate in the core region of the edge dislocation *-> higher stress is now required to move the dislocation* (*the system is in a low energy state after the segregation and higher stress is required to 'pull' the dislocation out of the energy well).*
- Defects associated with shear stress fields (having a non-spherical distortion field) can interact with the stress field of a screw dislocation.

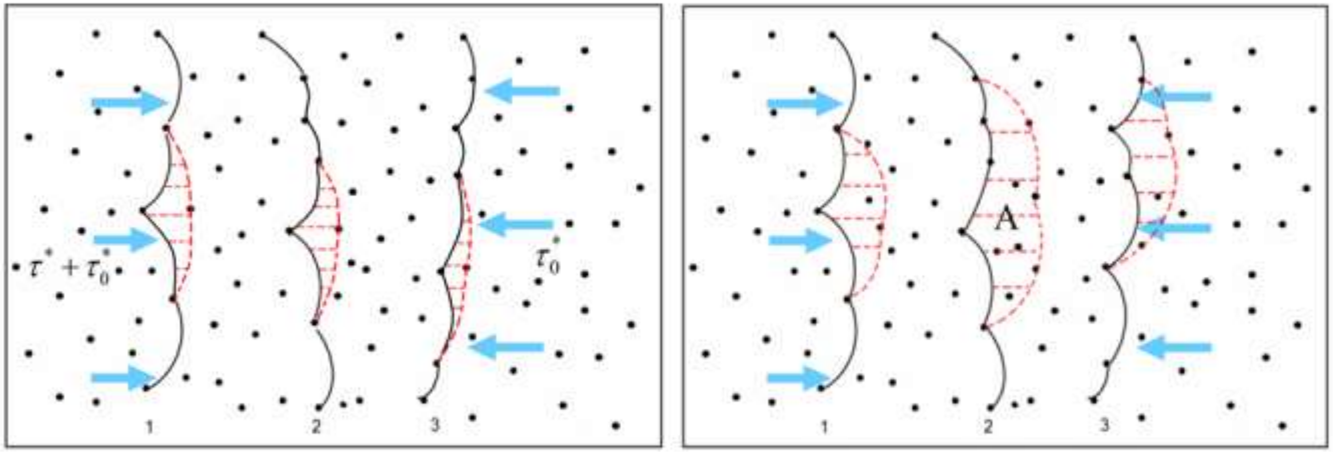
Dislocation-Point Defect Interactions

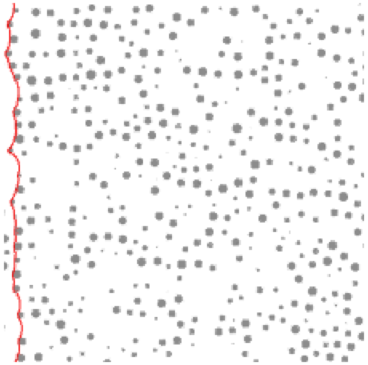
- Vacancies are attracted to the compressive regions of an edge dislocation and are repelled from tensile regions.
- The behavior of substitutional atoms smaller than the parent atoms is similar to that of the vacancies.
- Larger substitutional atoms are attracted to the tensile region of the edge dislocation and are repelled from the compressive regions.
- Interstitial atoms (associated with compressive stress fields) are attracted towards the tensile region of the edge dislocation and are repelled from the compressive region of the stress field.

Dislocation-Point Defect Interactions



Point Defect	Tensile Region	Compressive Region
Vacancy	Repelled	Attracted
Interstitial	Attracted	Repelled
Smaller substitutional atom	Repelled	Attracted
Larger Substitutional atoms	Attracted	Repelled

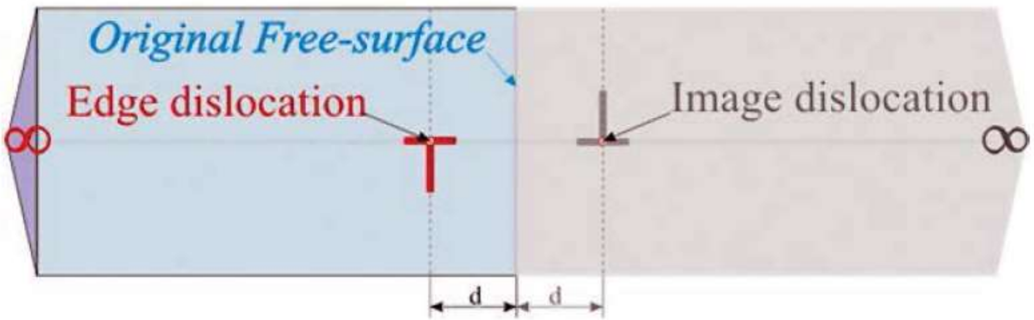

$\tau^* + \tau_0^*$
τ_0^*
1
2
3
A



Dislocation-surface Interactions

- Vacancies are attracted to the compressive regions of an edge dislocation and are repelled from tensile regions.
- A dislocation near a free surface experiences a force towards the free surface, which is called the image force.
- The force is called an ‘image force’ as the force can be calculated assuming an negative hypothetical dislocation on the other side of the surface. The attractive force between the dislocations (+ & □) is gives the image force.
- If the image force exceeds the Peierls stress, then the dislocation can leave the crystal spontaneously without application of external stresses!
- Hence, regions near a free surface or nano-crystals can become spontaneously dislocation free. In nanocrystals due to the proximity of more than one surface, many images have to be constructed and the net force is the superposition of these image forces.

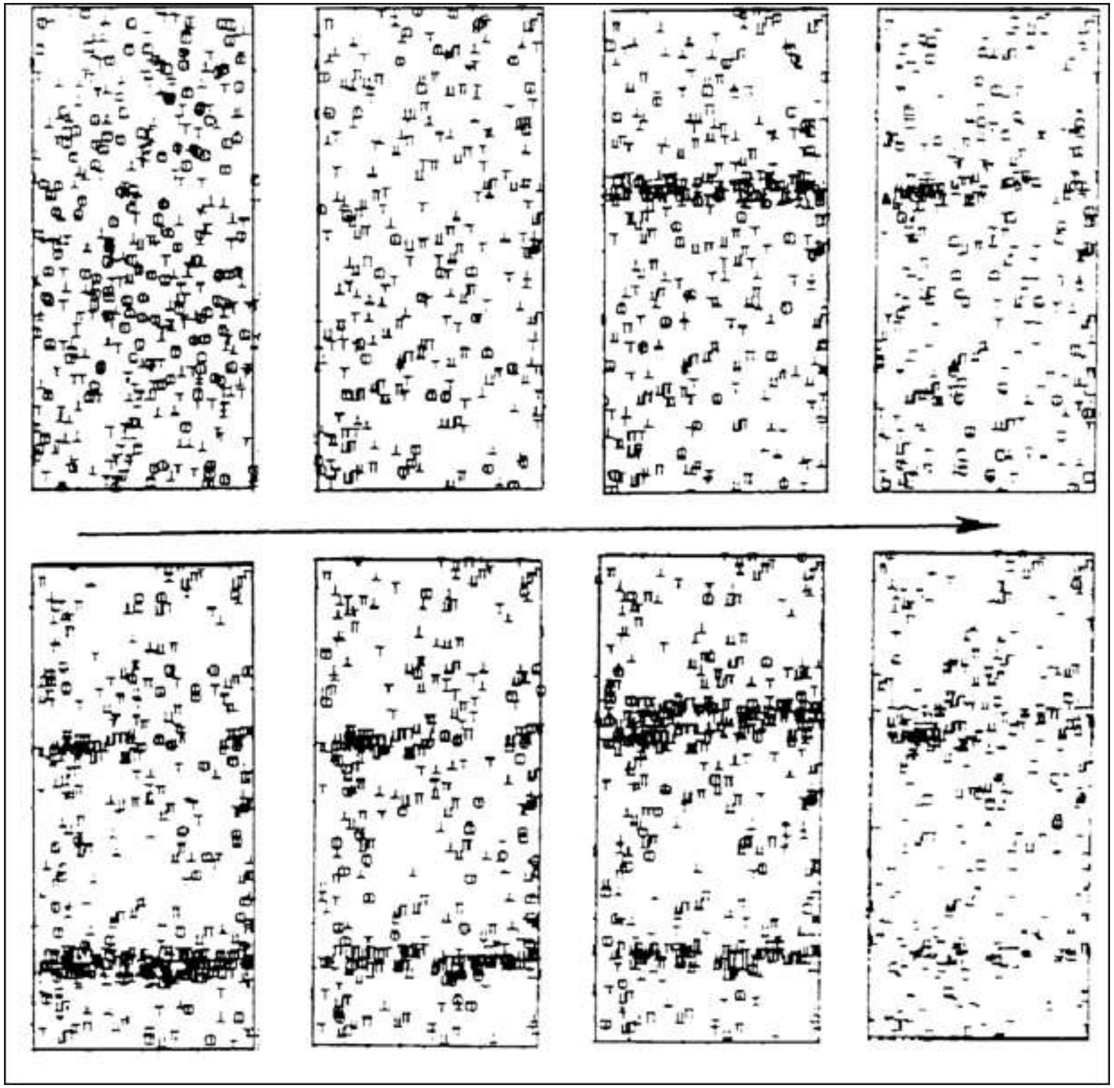
Dislocation-surface Interactions



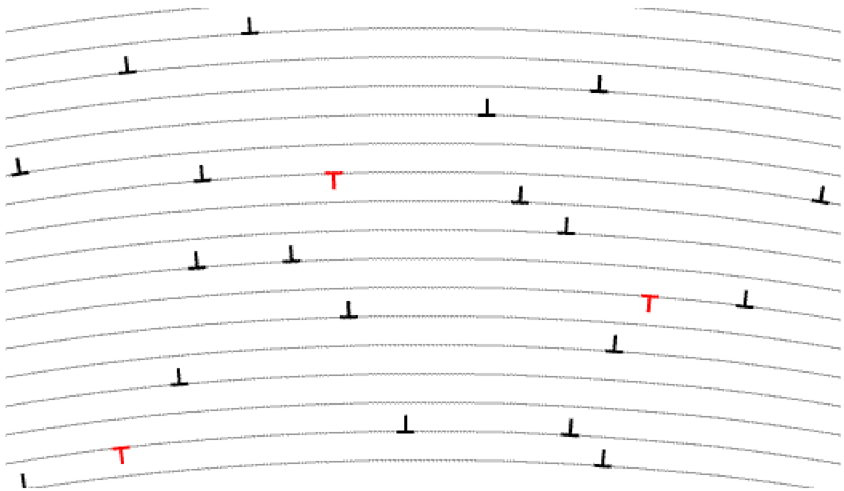
$$F_{image} = \frac{-Gb^2}{4\pi(1-\nu)d}$$

Examples

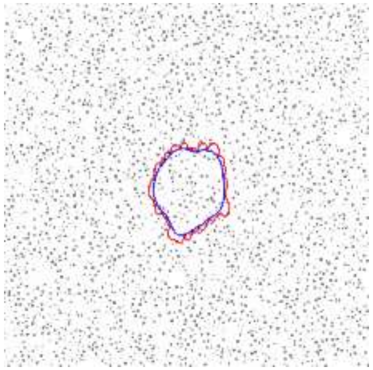
Example of Discrete Dislocation Dynamics in 2D



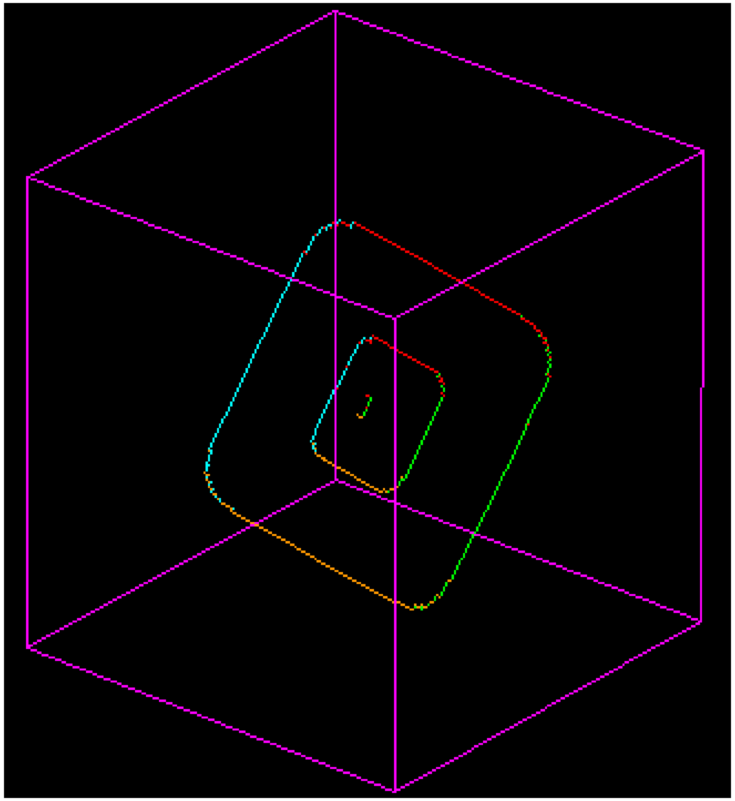
Example of Discrete Dislocation Dynamics in 2D



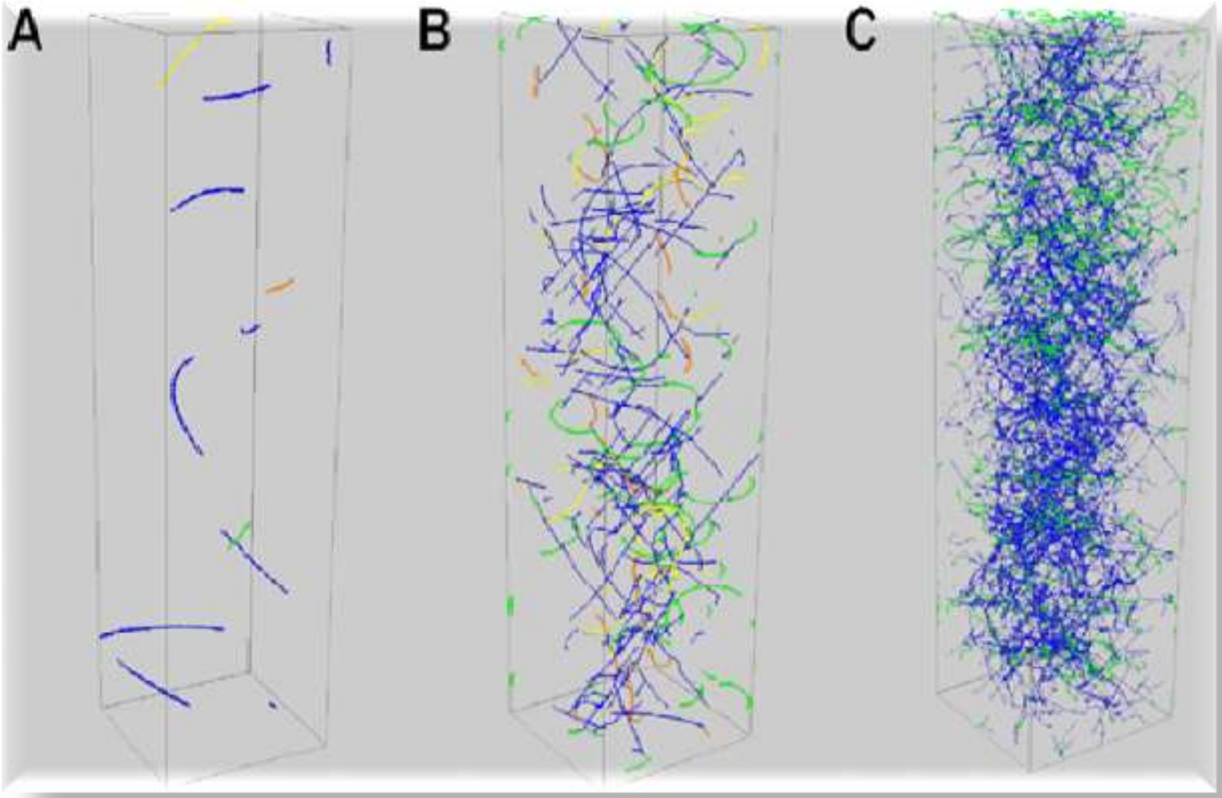
Example of Discrete Dislocation Dynamics in 2D



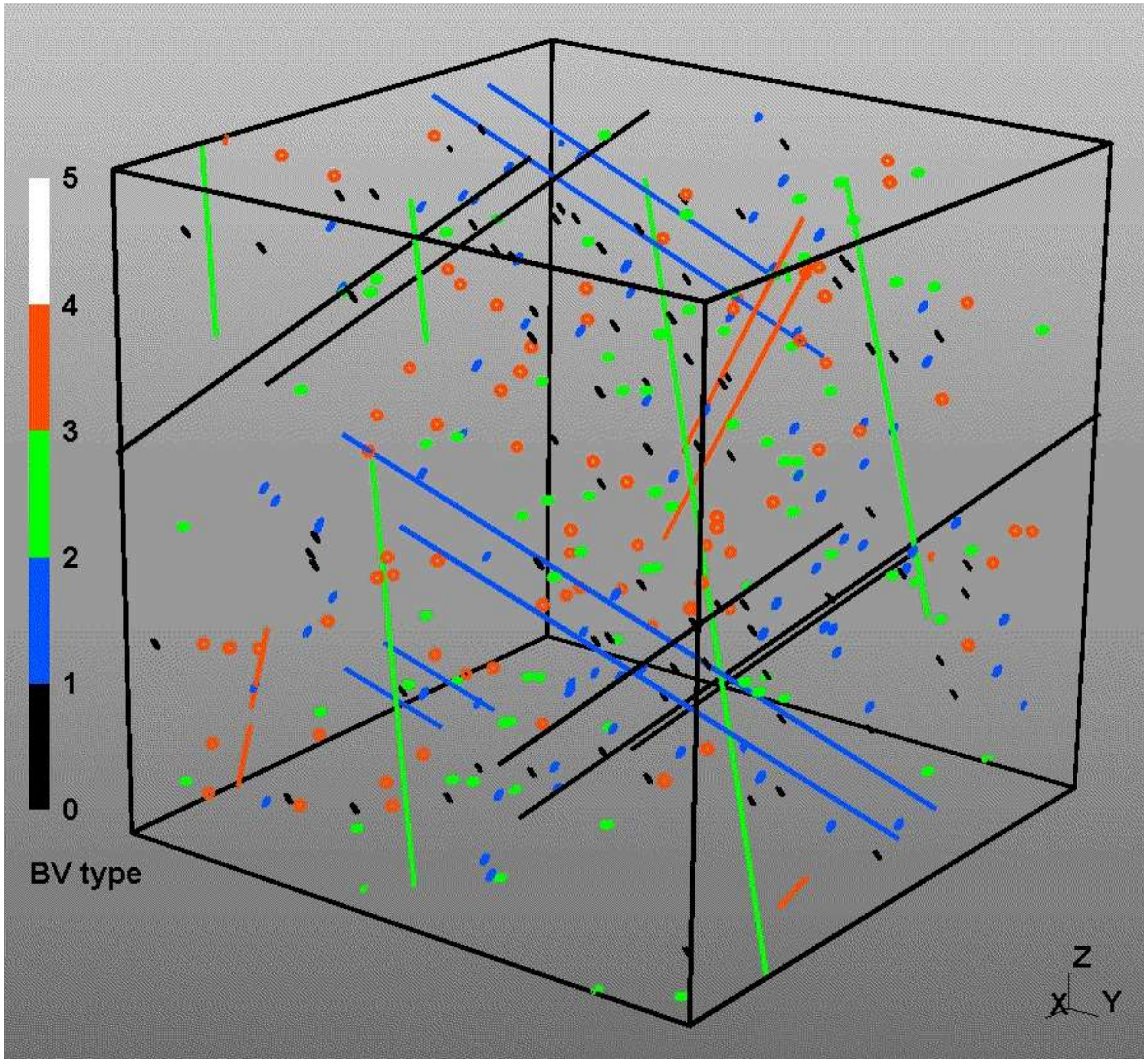
Example of Discrete Dislocation Dynamics in 3D



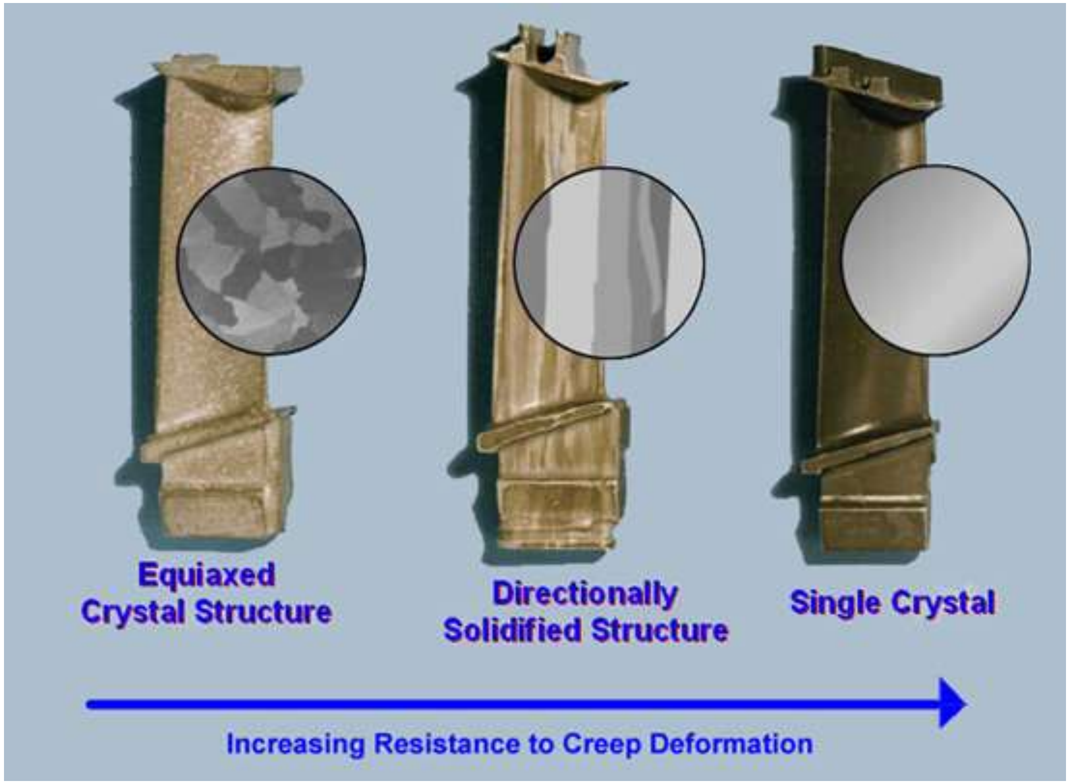
Example of Discrete Dislocation Dynamics in 3D



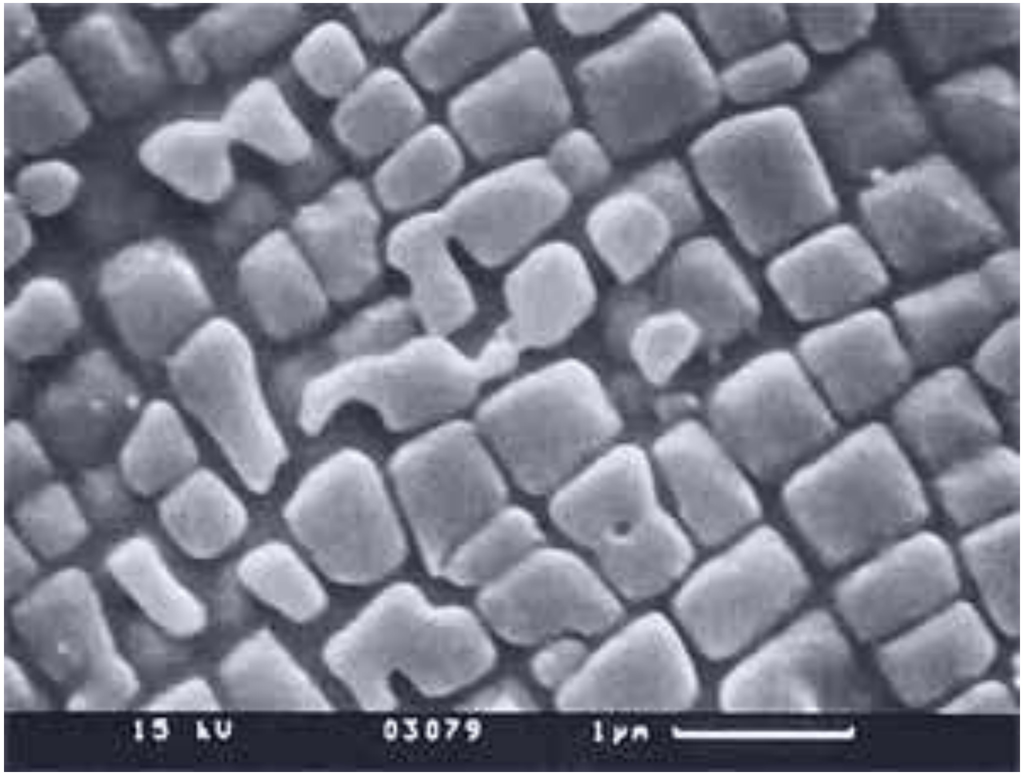
Example of Discrete Dislocation Dynamics in 3D



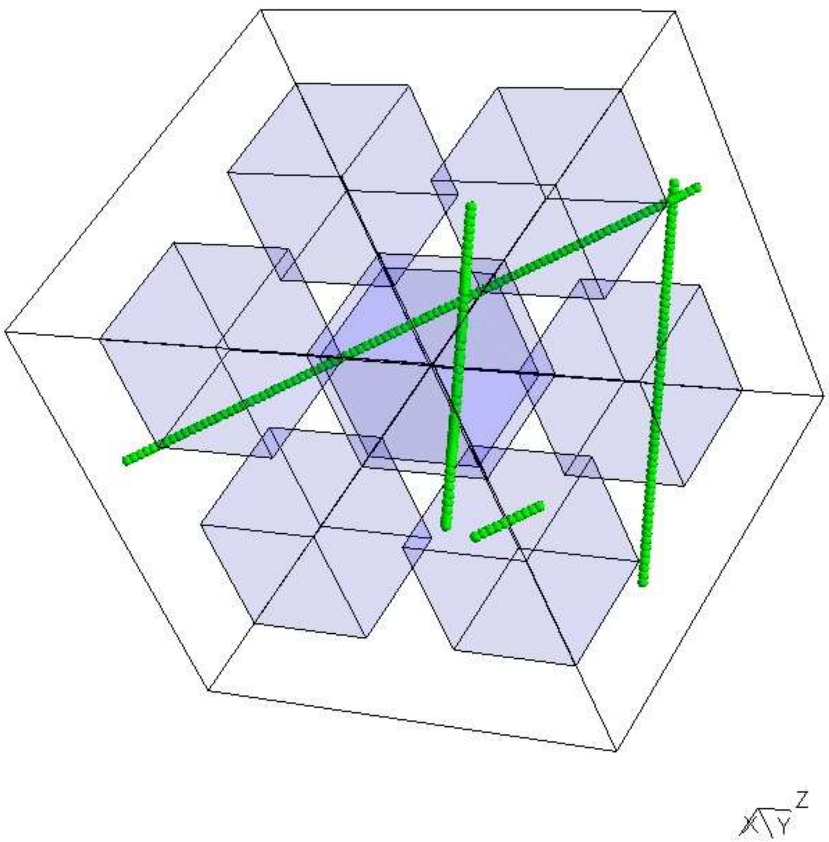
Example of Discrete Dislocation Dynamics in 3D: superalloys

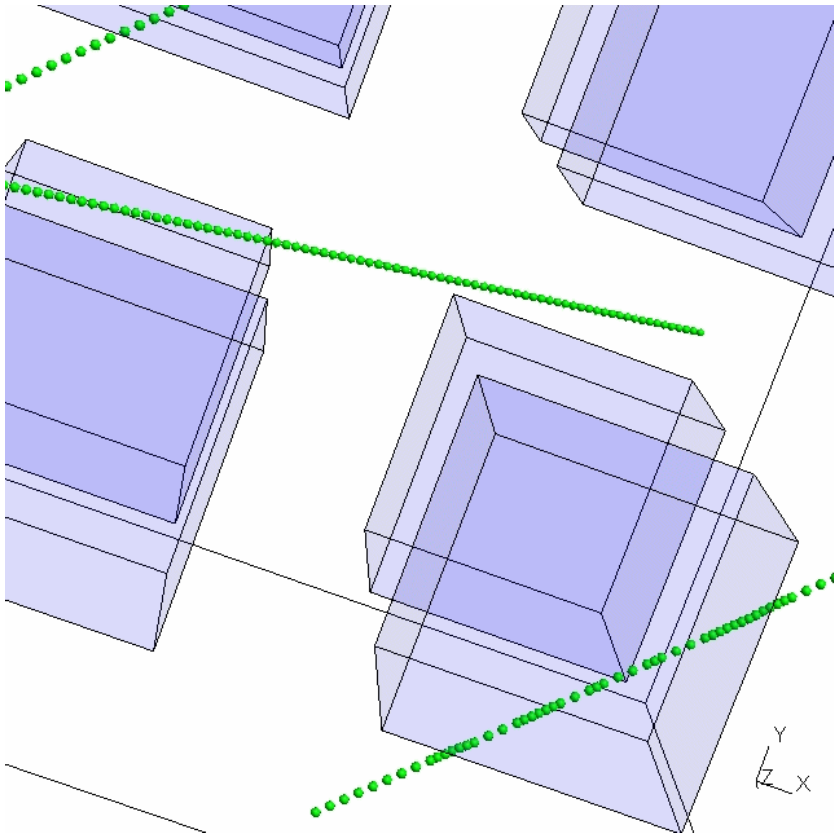


Example of Discrete Dislocation Dynamics in 3D: superalloys

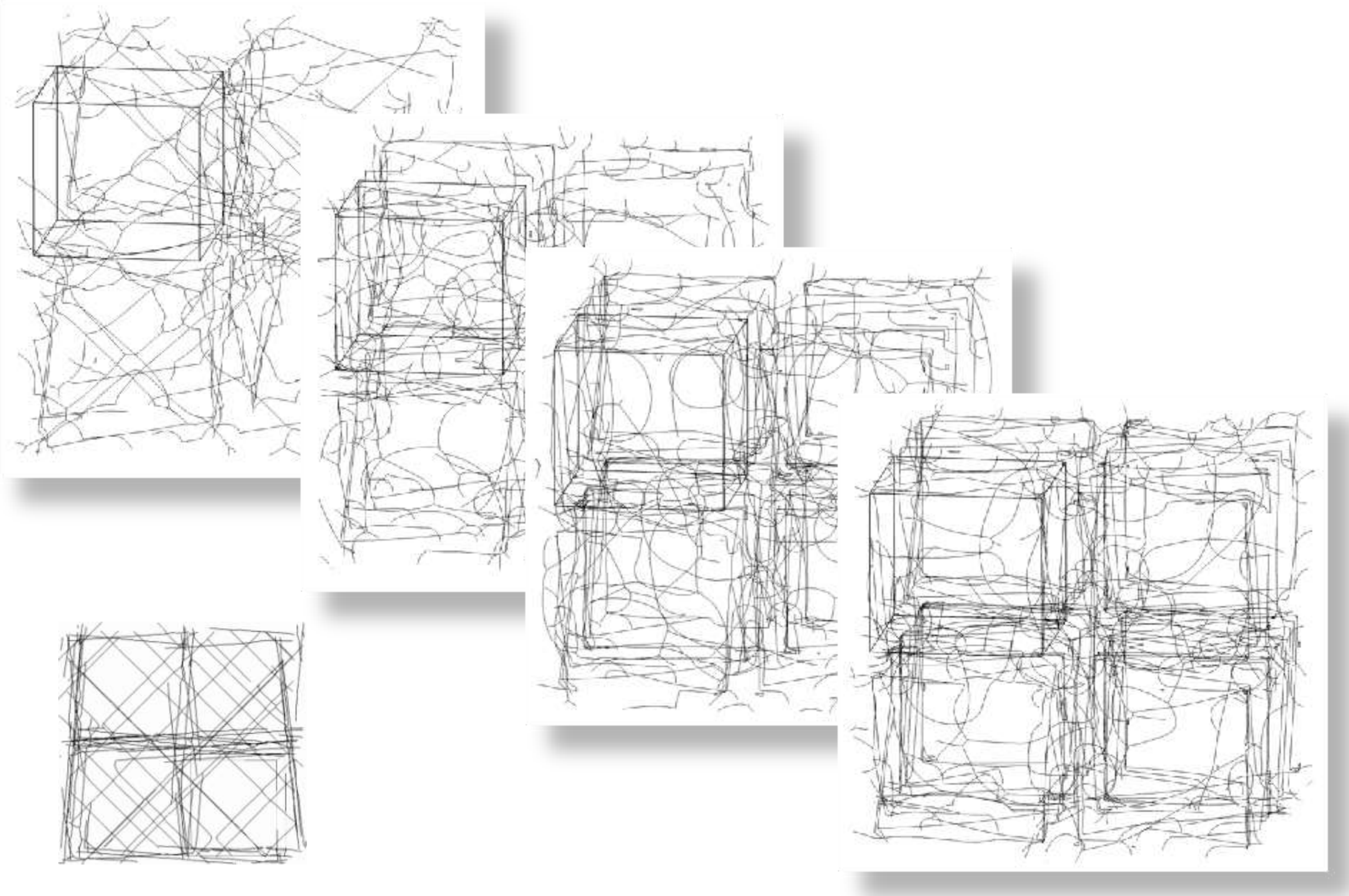


Example of Discrete Dislocation Dynamics in 3D

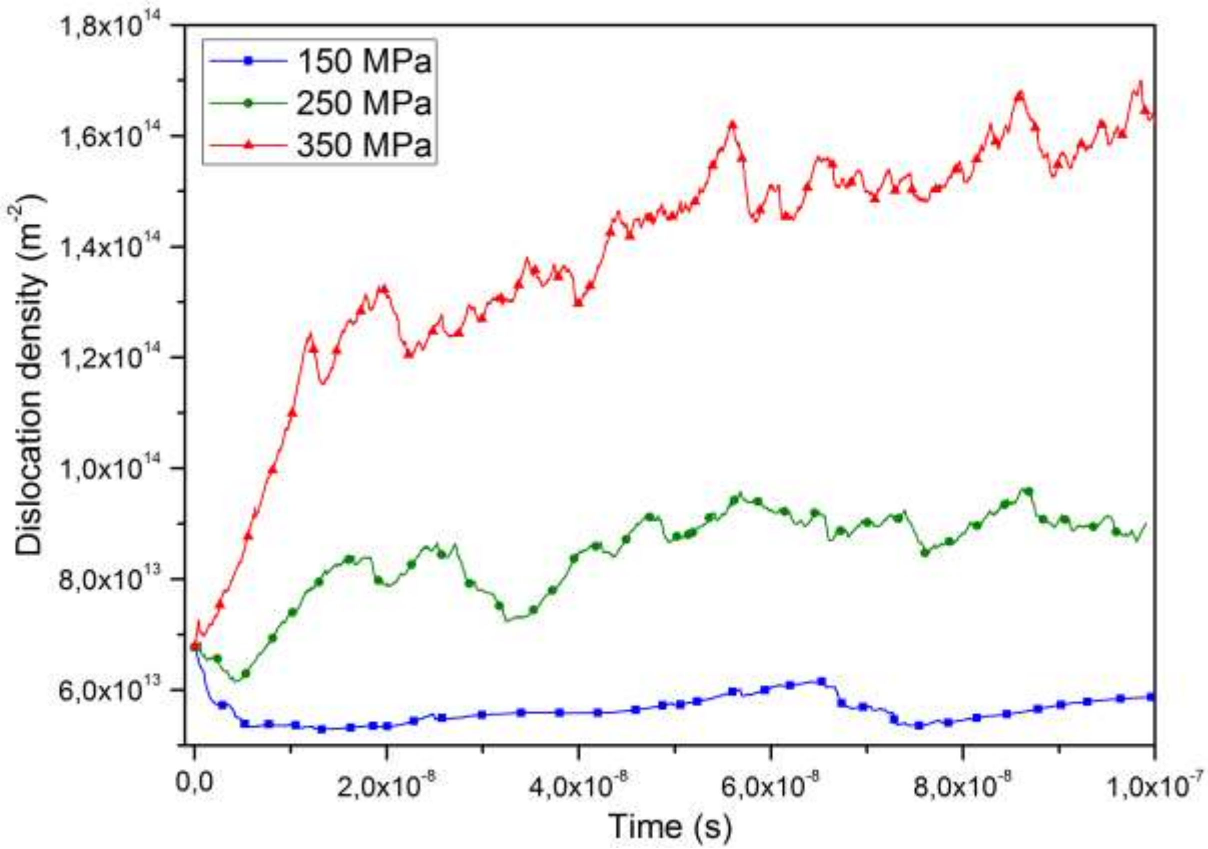




Example of Discrete Dislocation Dynamics in 3D: superalloys

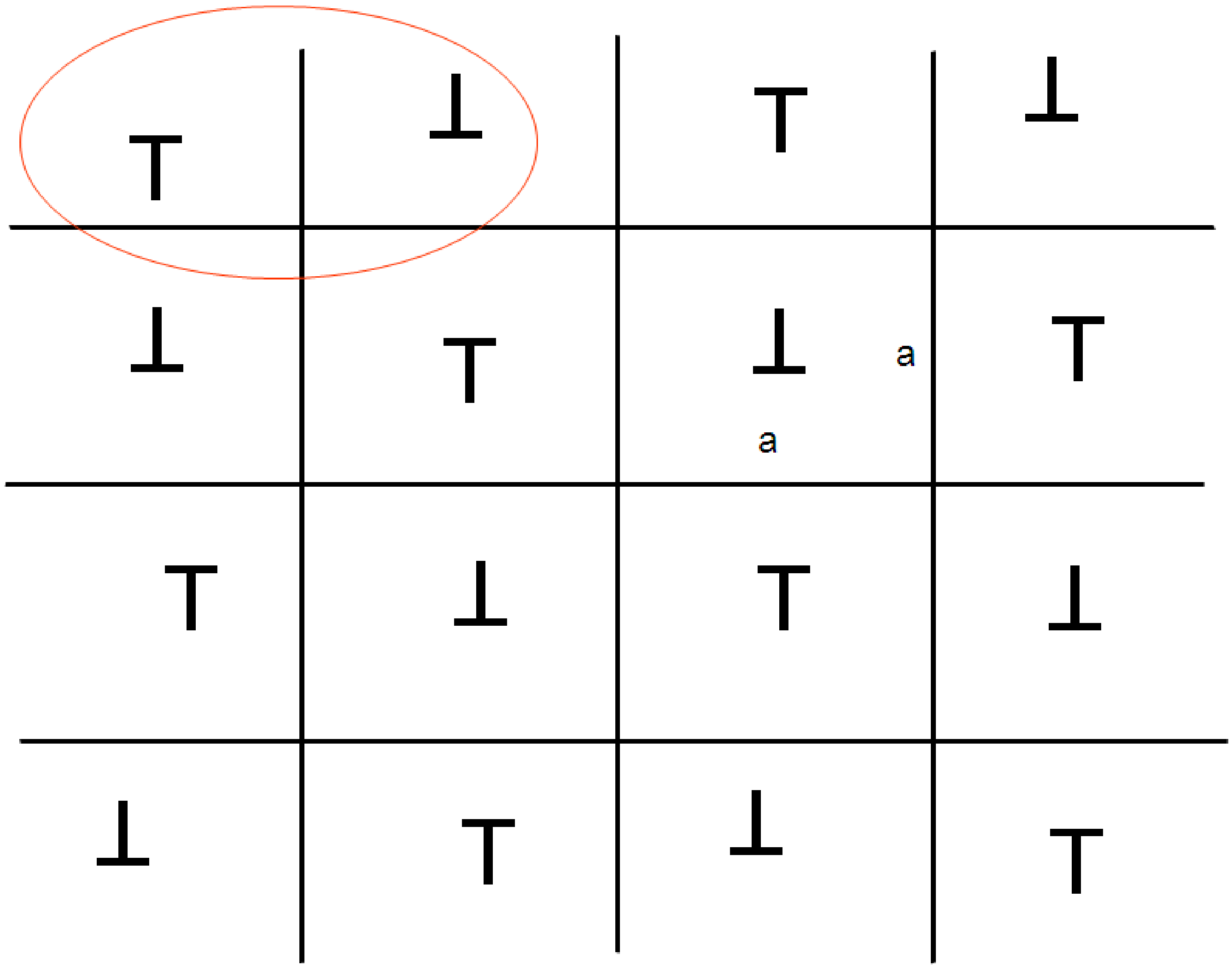


Example of Discrete Dislocation Dynamics in 3D: superalloys



WHY Statistical Dislocation Dynamics ?

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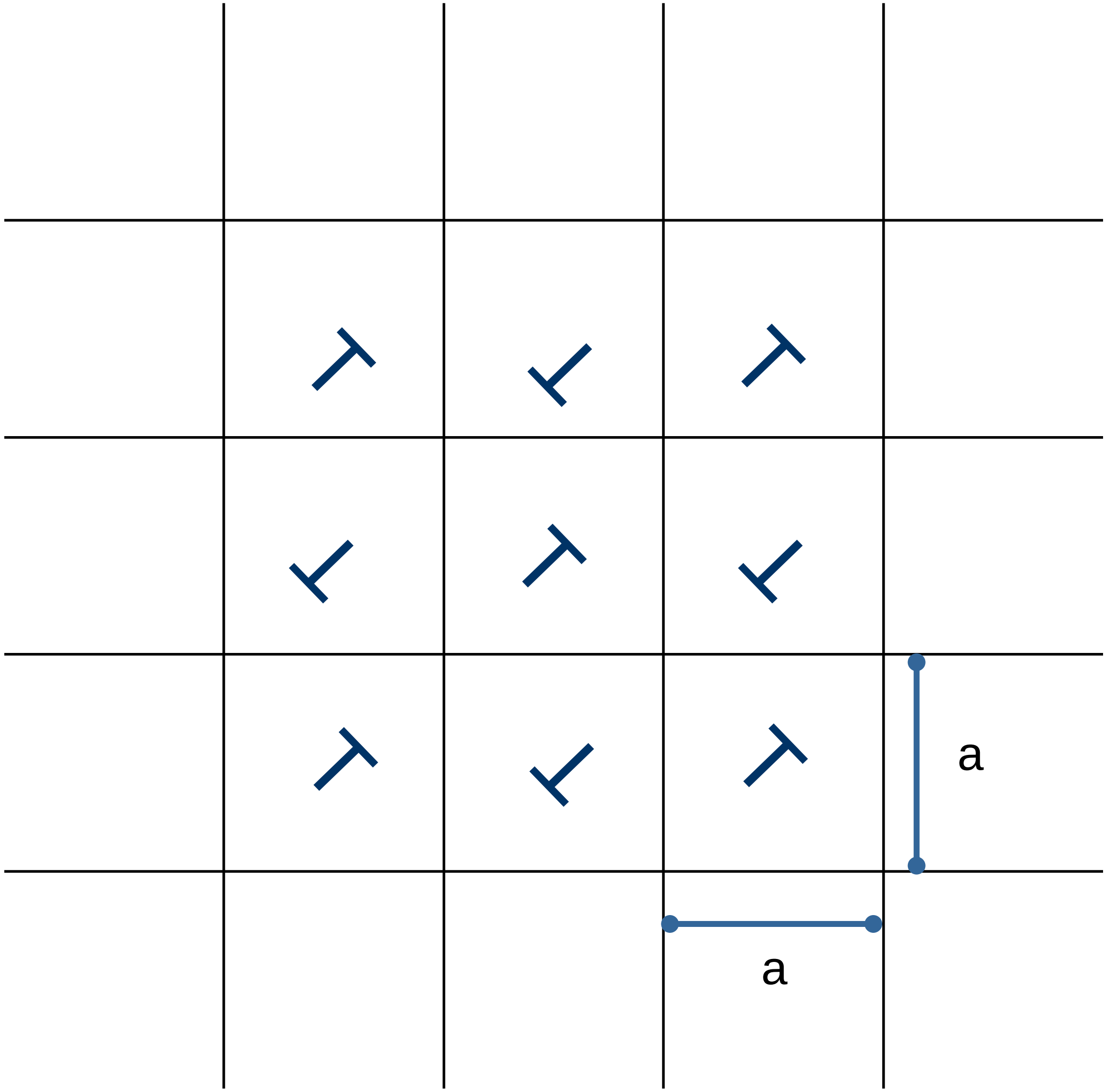
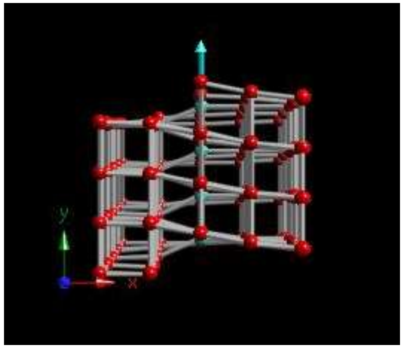


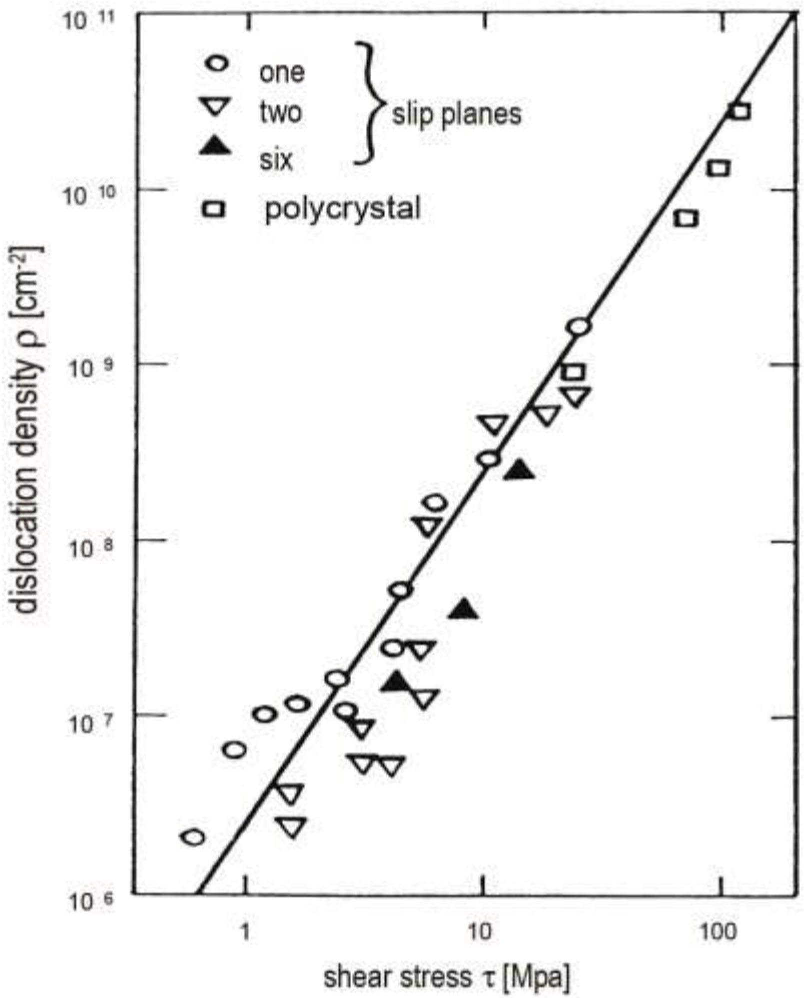


$$\tau = G\gamma = \frac{Gb}{2\pi\, r}$$

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

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

- kinetic equation of state

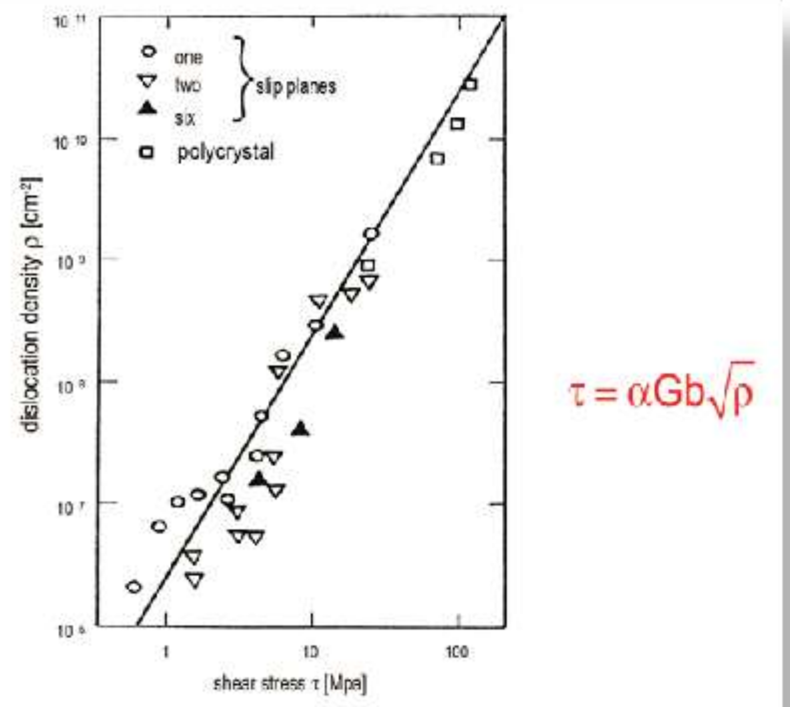


$$\tau = \alpha G b \sqrt{\rho}$$

Statistical Dislocation Dynamics

<u>kinetics</u>: collective dislocation behaviour

- kinetic equation of state

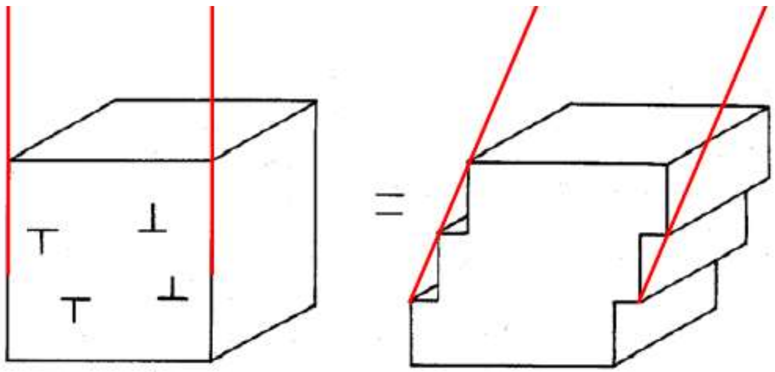


$$\tau = \alpha G b \sqrt{\rho}$$

- structure evolution

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

- coupling to imposed shape change



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