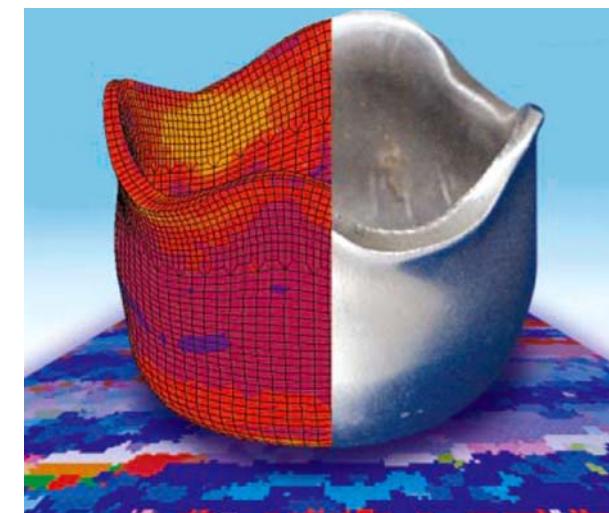
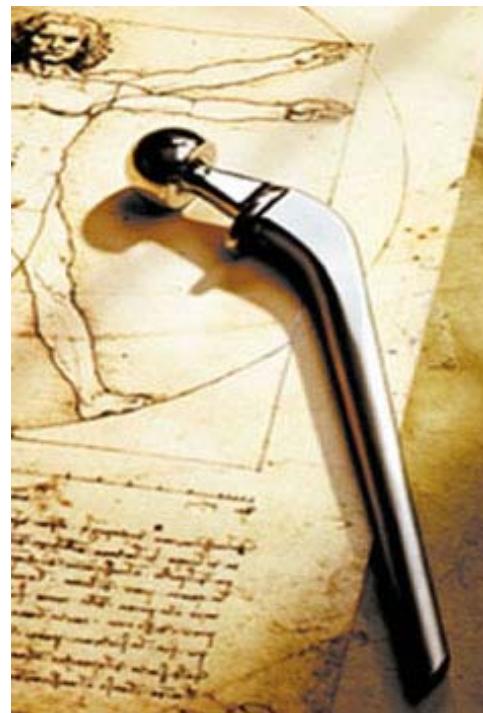


# Class 2007

lecture notes, spring 2007  
Prof. Dr. Dierk Raabe  
*Max-Planck-Institut*  
*Düsseldorf*



idea of this class:

repeat structure and dislocation statics

learn more about dislocation dynamics

learn crystal mechanics (more complex boundary conditions)

learn polymer crystal mechanics

learn some bio-materials science

focus on: structure and mechanics, crystallographic mat. sc.

email:  
[d.raabe@mpie.de](mailto:d.raabe@mpie.de)

Your email (capable for larger attachments)

lecture download page: [www.mpie.de](http://www.mpie.de)

class times:

.....

some test question during class

slides will be placed on the mpie website

## **further reading:**

basic things: any textbook on mater. science such as:

- Gottstein
- Hirth
- Physical Metallurgy Principles by Reed-Hill
- Elementary Dislocation Theory, J. Weertman and J.R. Weertman, Oxford University Press (1992).  
Reprint of 1964 classic
- Introduction to Dislocations, D. Hull and D.J. Bacon, Butterworth-Heinemann Ltd.

advanced crystal mechanics:

- W. F. Hosford, The Mechanics of Crystals and Textured Polycrystals, Oxford University Press (1993).
- Kocks, U. F., Tomé, C., Wenk, H.-R., 1997. Texture and Anisotropy. Preferred Orientations in Polycrystals and Their Effect on Material Properties. Cambridge University Press, Cambridge, England.
- D. Raabe, F. Roters, F. Barlat, L.-Q. Chen (eds.), Wiley-VCH, Weinheim, Juni 2004, ISBN 3-527-30760-5
- „Continuum Scale Simulation of Engineering Materials - Fundamentals - Microstructures - Process Applications“

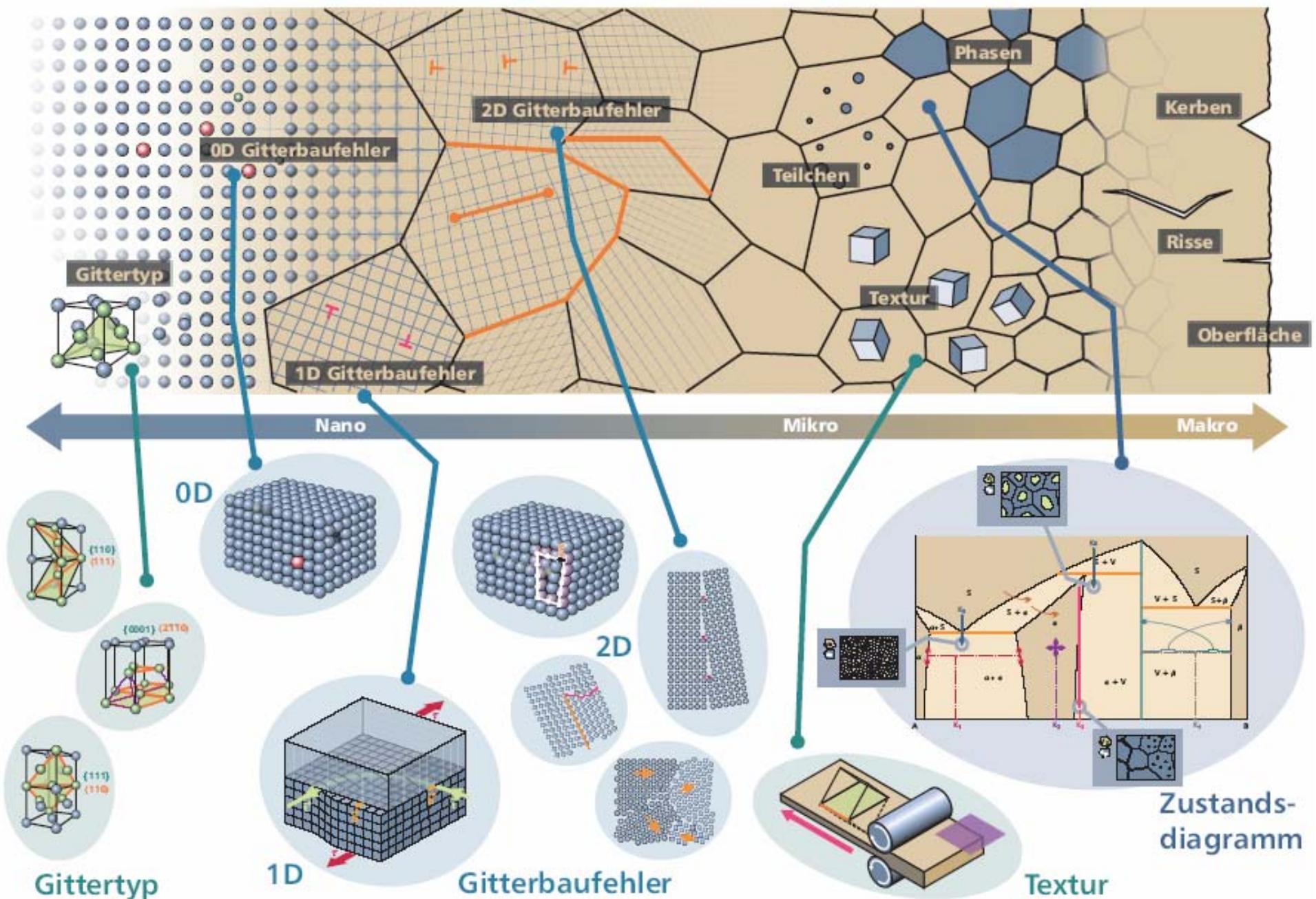
# Contents

- **What is microstructure ?**
- **Crystal structure**
- **Dislocations**
- **Single crystal and polycrystal mechanics**
- **Partially-crystalline materials (polymers)**
- **Micromechanics of biomaterials and biological materials**

## **What is microstructure ?**

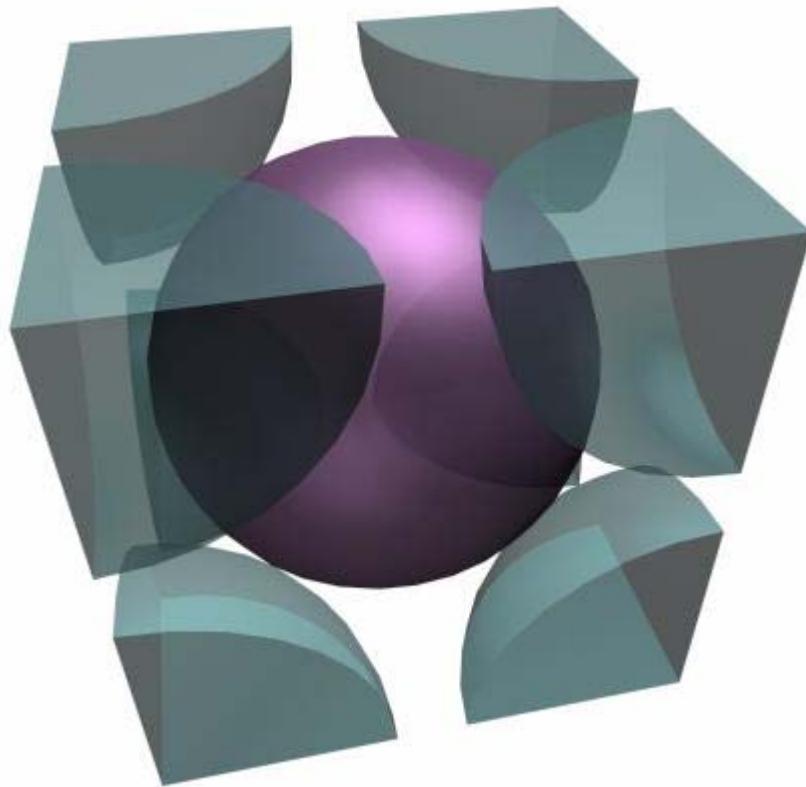
**All non-equilibrium lattice defects**

**here: focus on crystals, crystal mechanics  
and anisotropy**



# Crystal structure

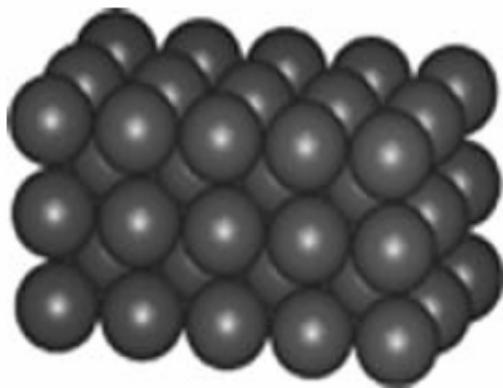
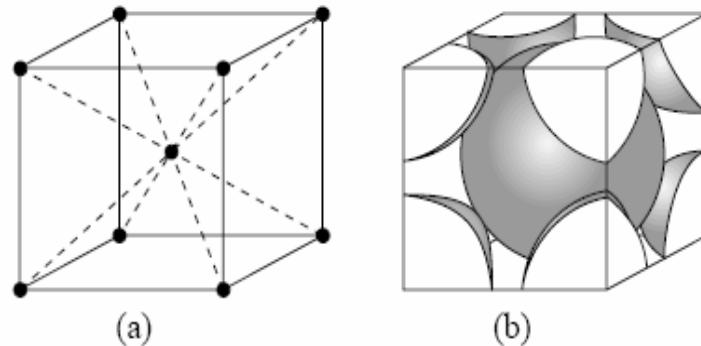
anisotropy at the  
lattice cell level



**BCC**

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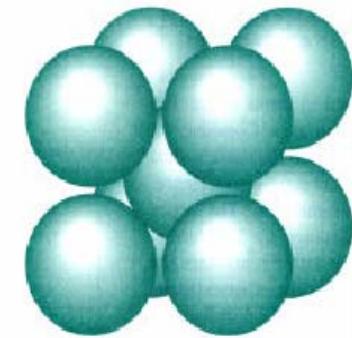
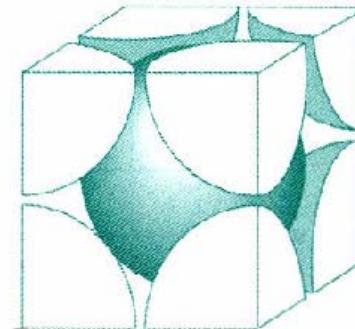
# Fe ( $\alpha$ ), Cr, Mo, Ta, Nb, Mo, W



**BCC**

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

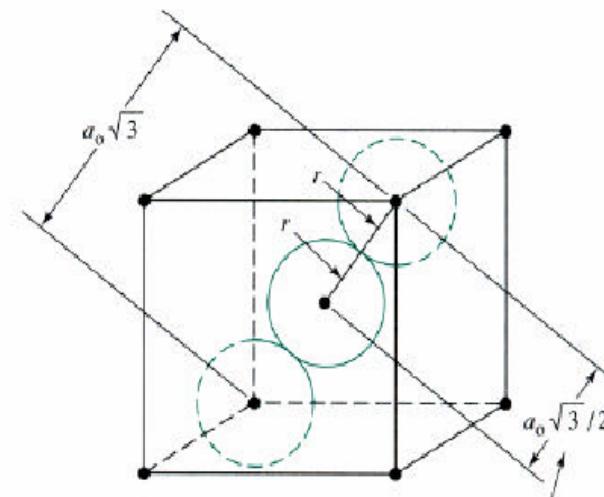
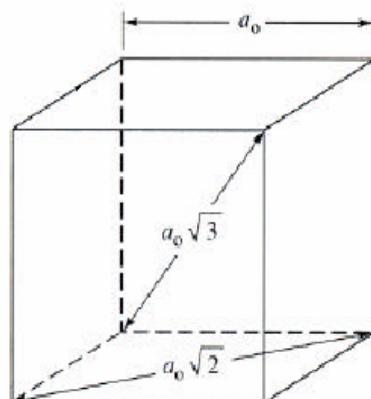


$$\text{coordination number} = 4 + 4 = 8$$

$$\text{atomic packaging} = 0.68$$

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

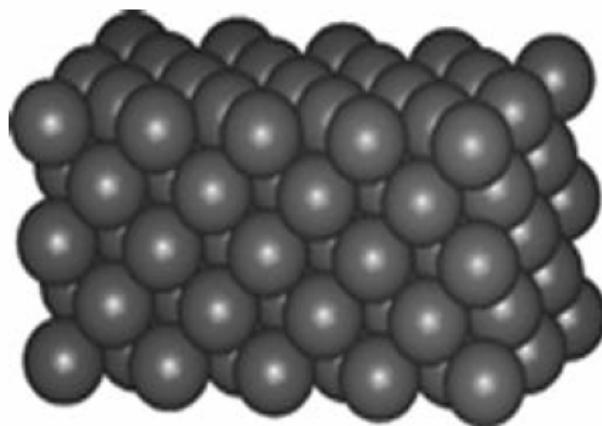
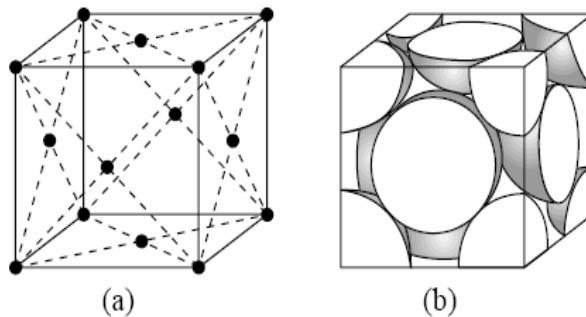
$$a = \frac{4}{\sqrt{3}}r$$



BCC

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# Fe ( $\gamma$ ), Al, Cu, Au



FCC

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atoms per cell

$$= (8 \times 1/8) + (6 \times 1/2) = 4$$

coordination number

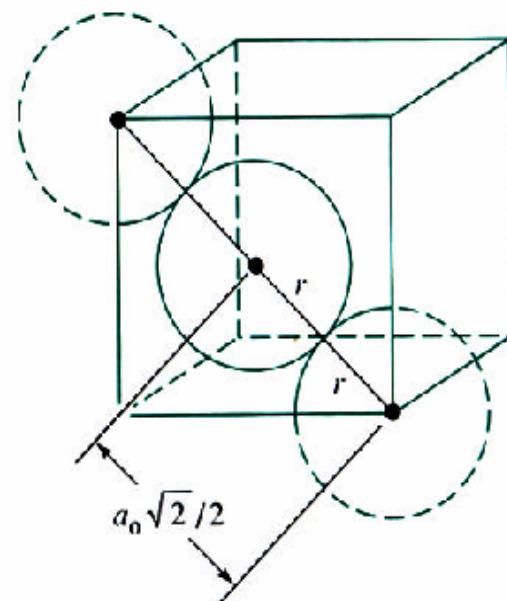
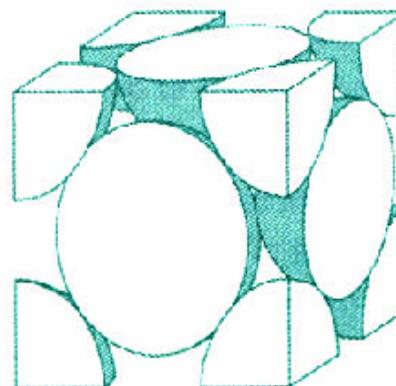
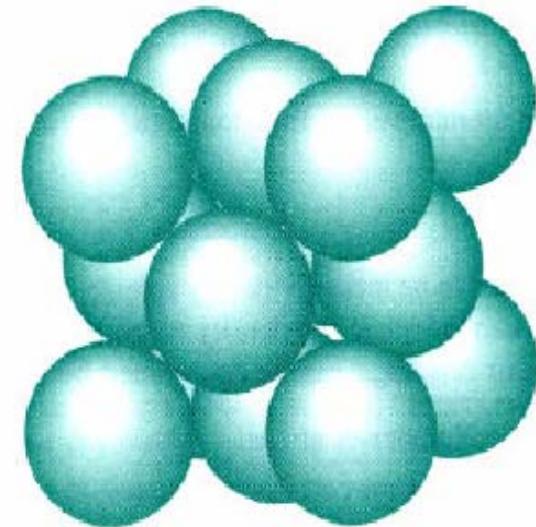
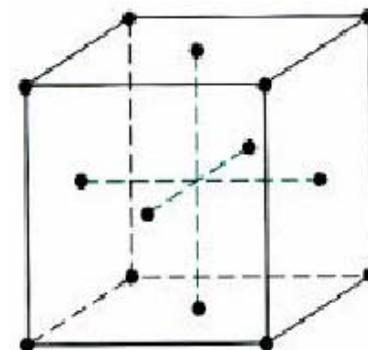
$$= 4 + 4 + 4 = 12$$

atomic packaging

$$= 0.74$$

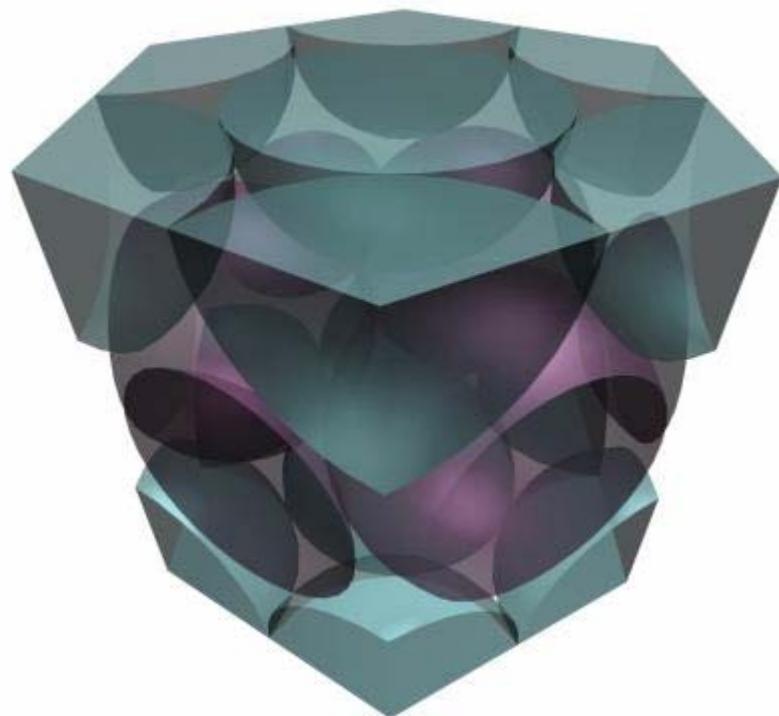
$$4r = \sqrt{2}a$$

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



FCC

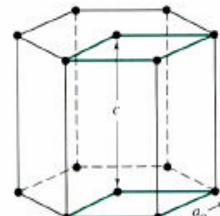
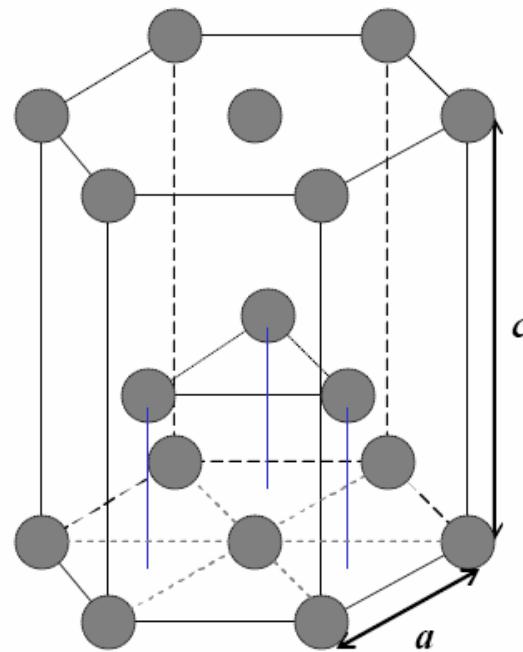
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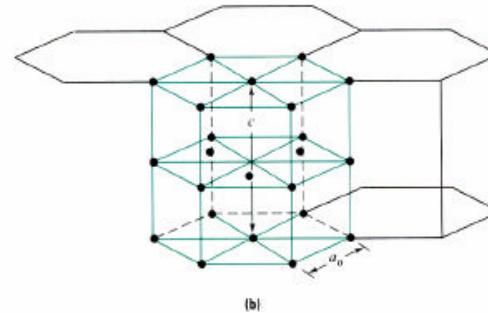
**hexagonal**

### 3. HCP: hexagonal close-packed

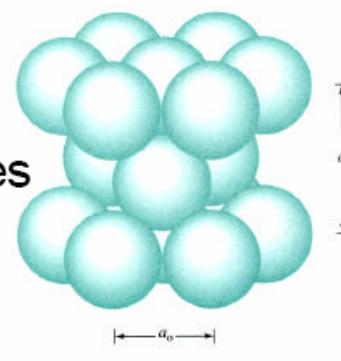
(Mg, Be, Co, Ti, Zn)



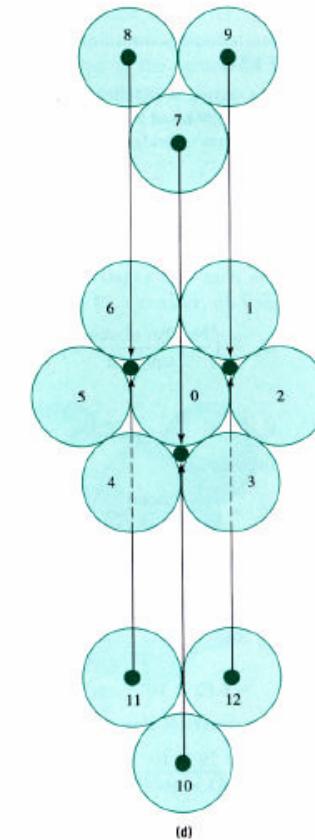
(a)



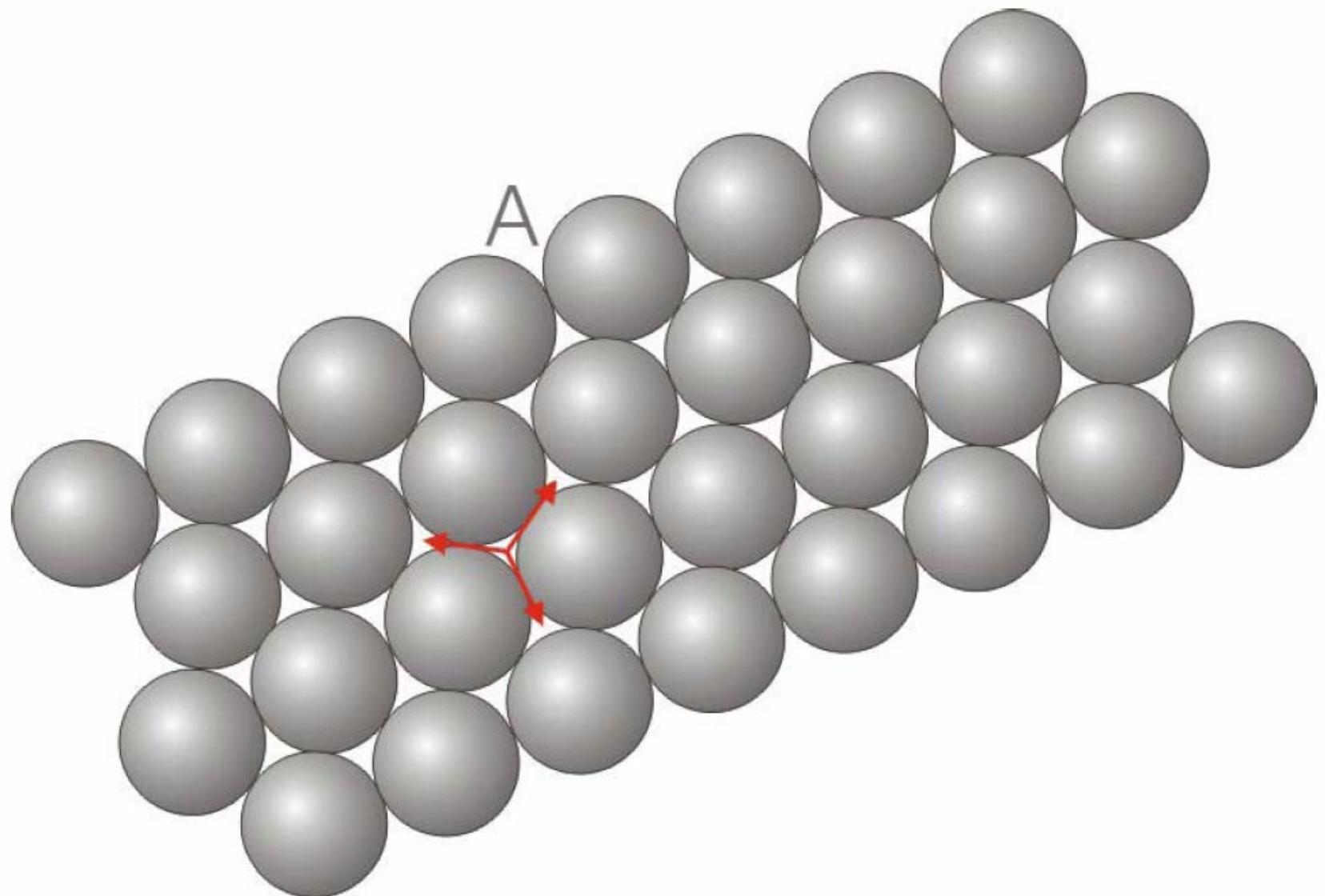
(b)

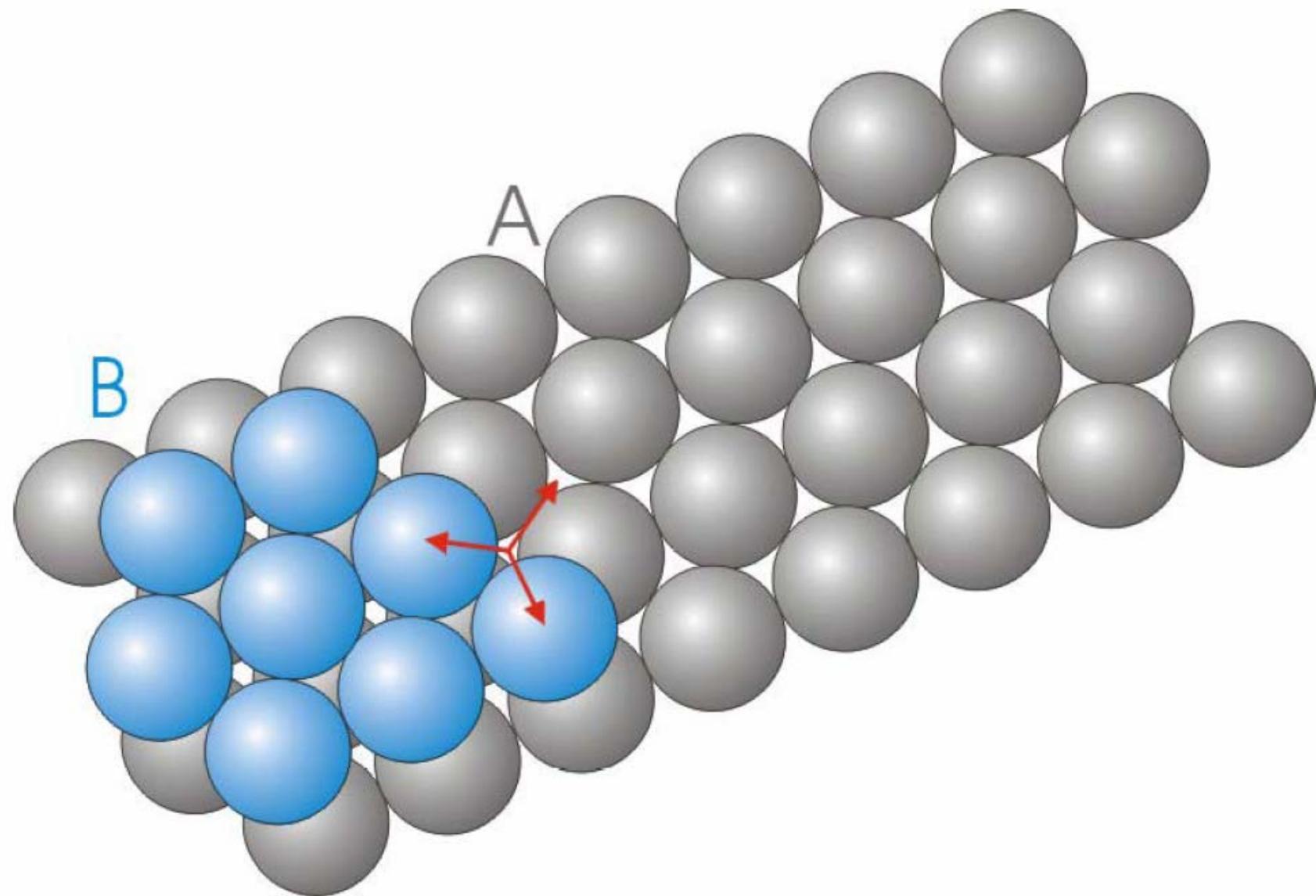


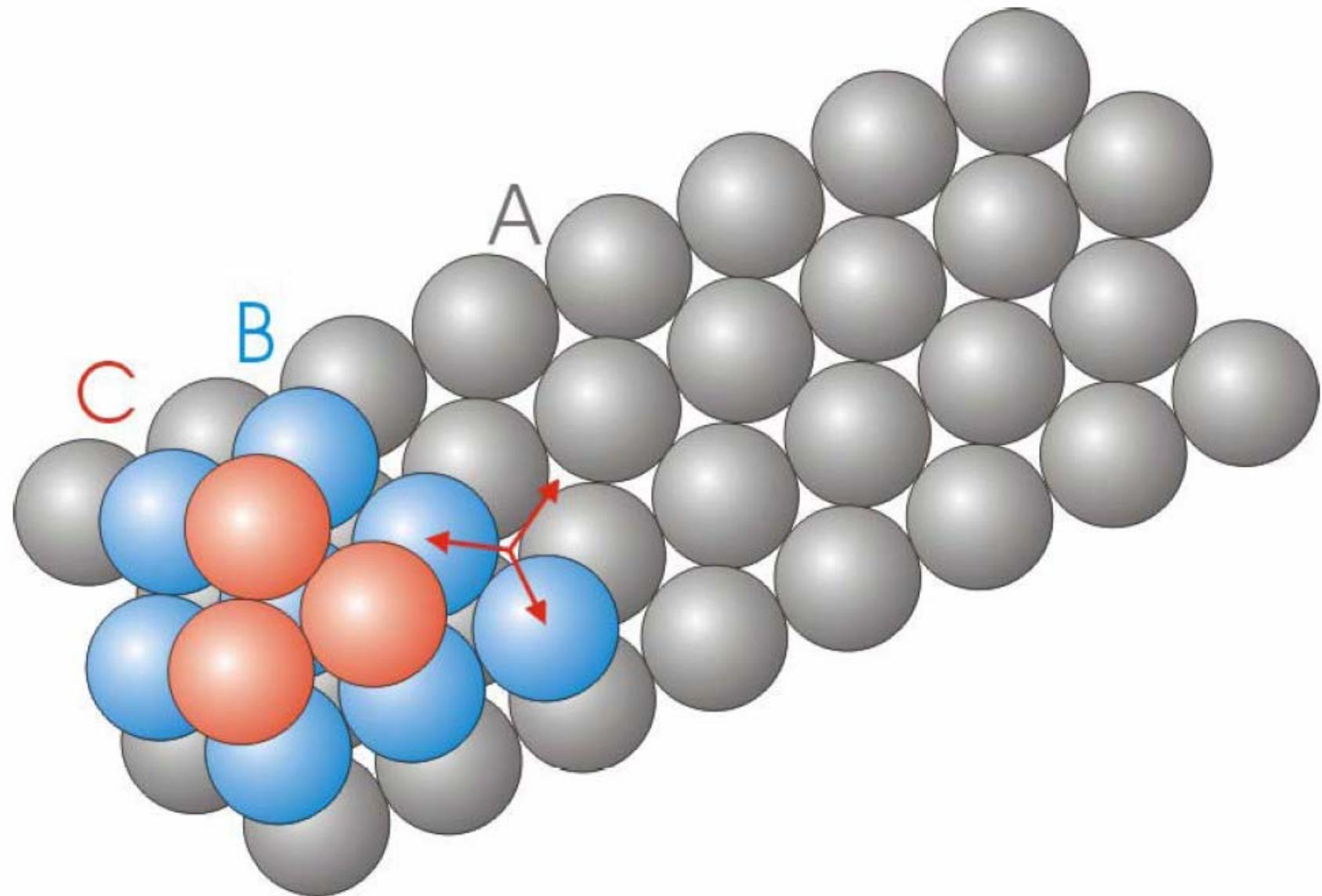
noncubic symmetry: **a** and **c** axes  
 $c/a \sim 1.633$

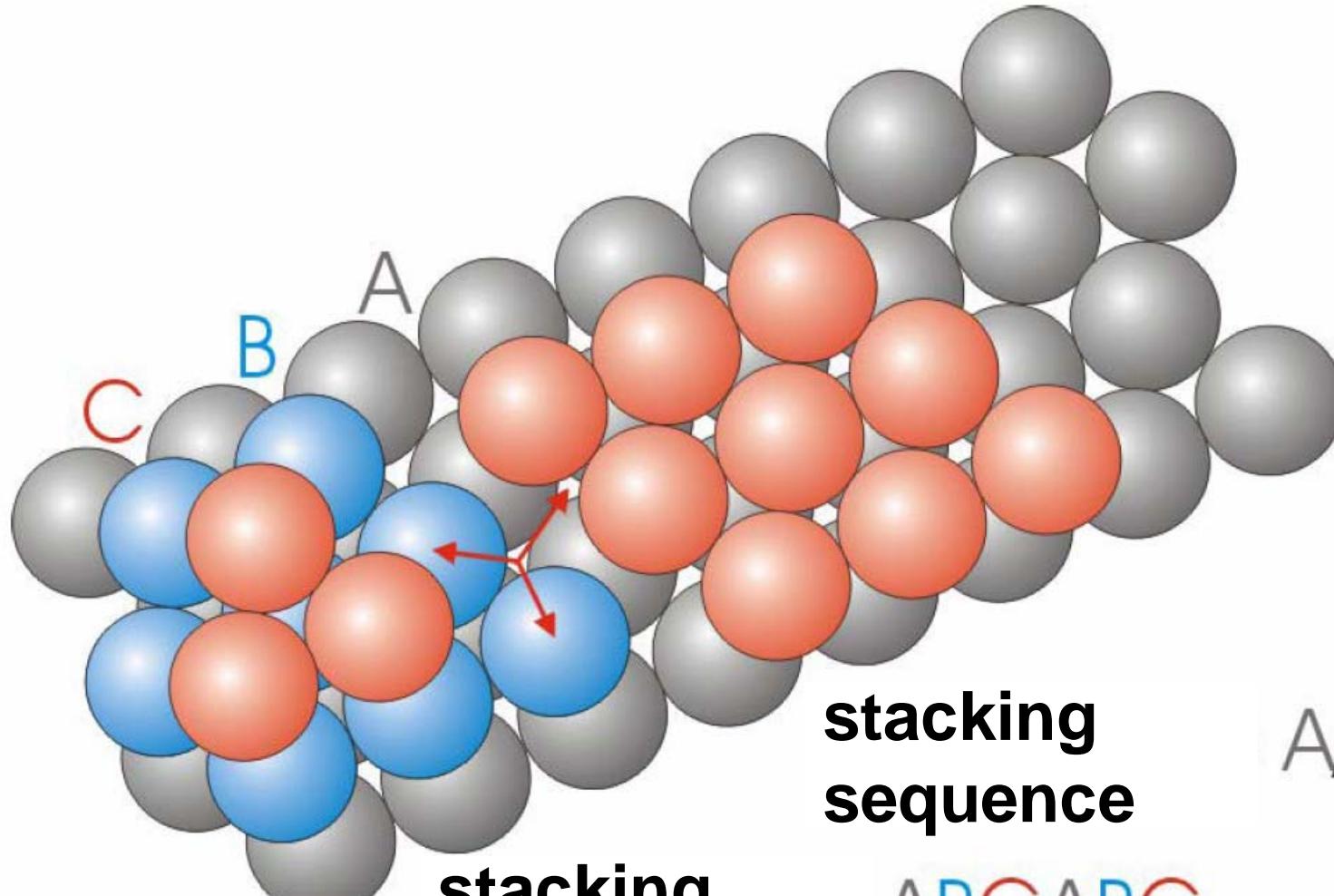


hexagonal









stacking  
sequence

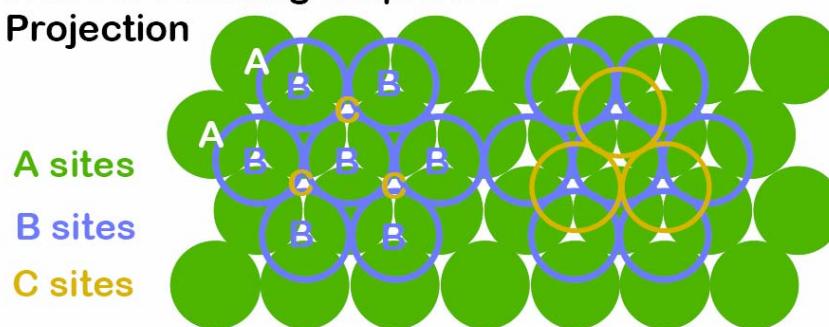
stacking  
sequence

ABCABC

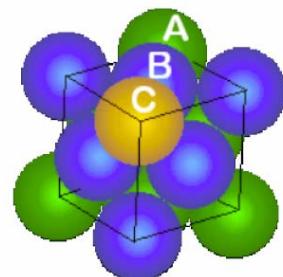
A/CABC

## FCC STACKING SEQUENCE

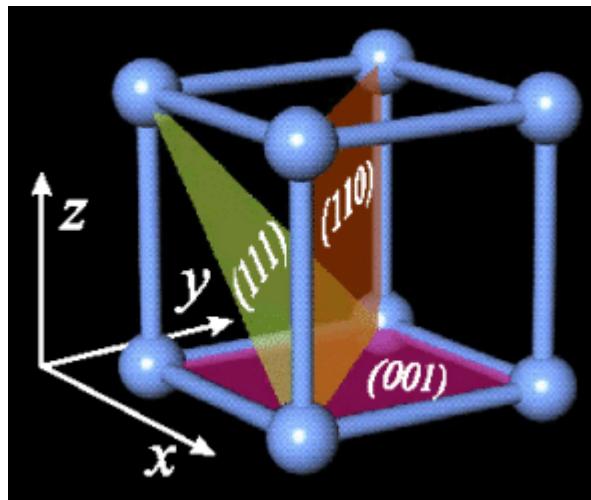
- ABCABC... Stacking Sequence
- 2D Projection

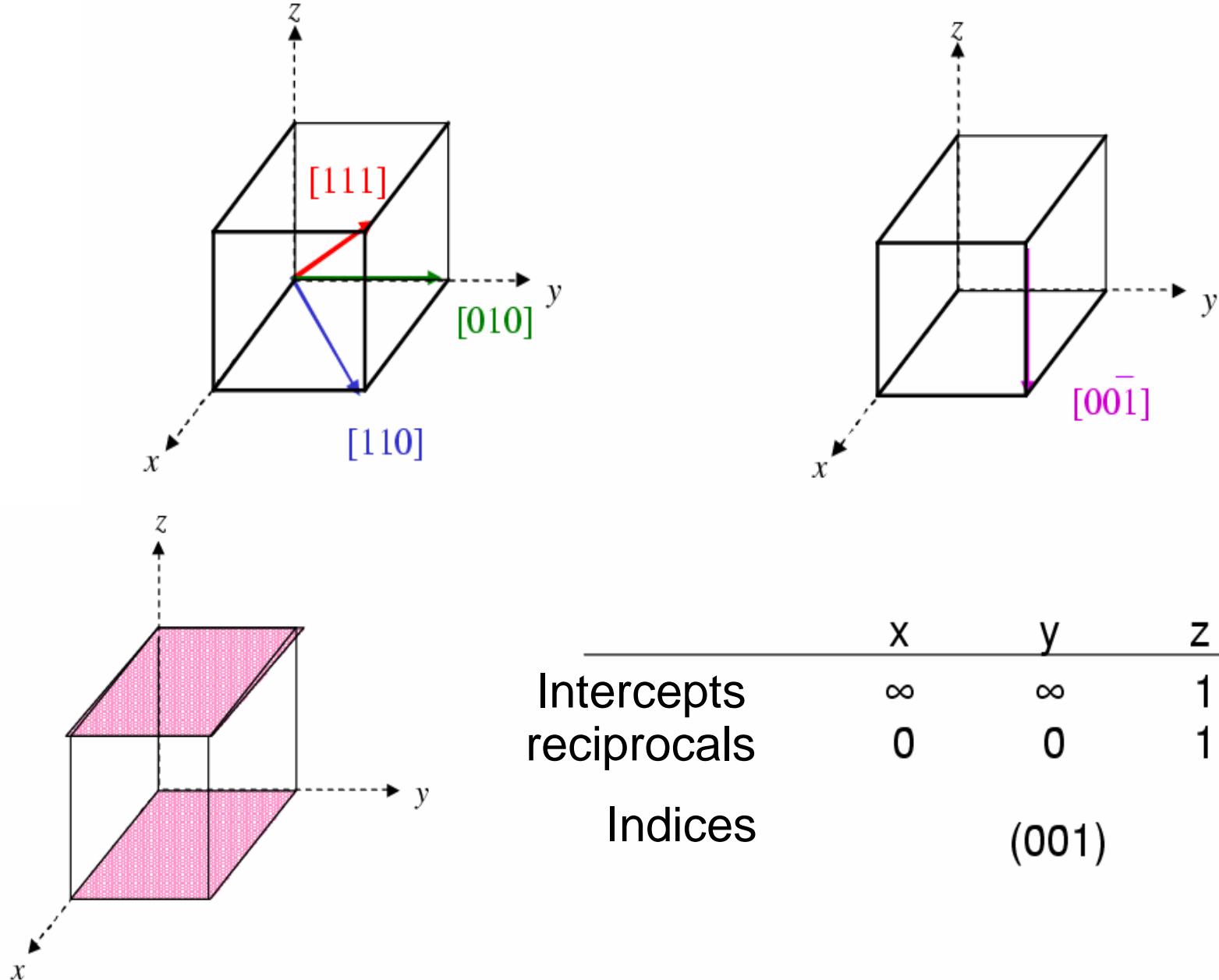


- FCC Unit Cell



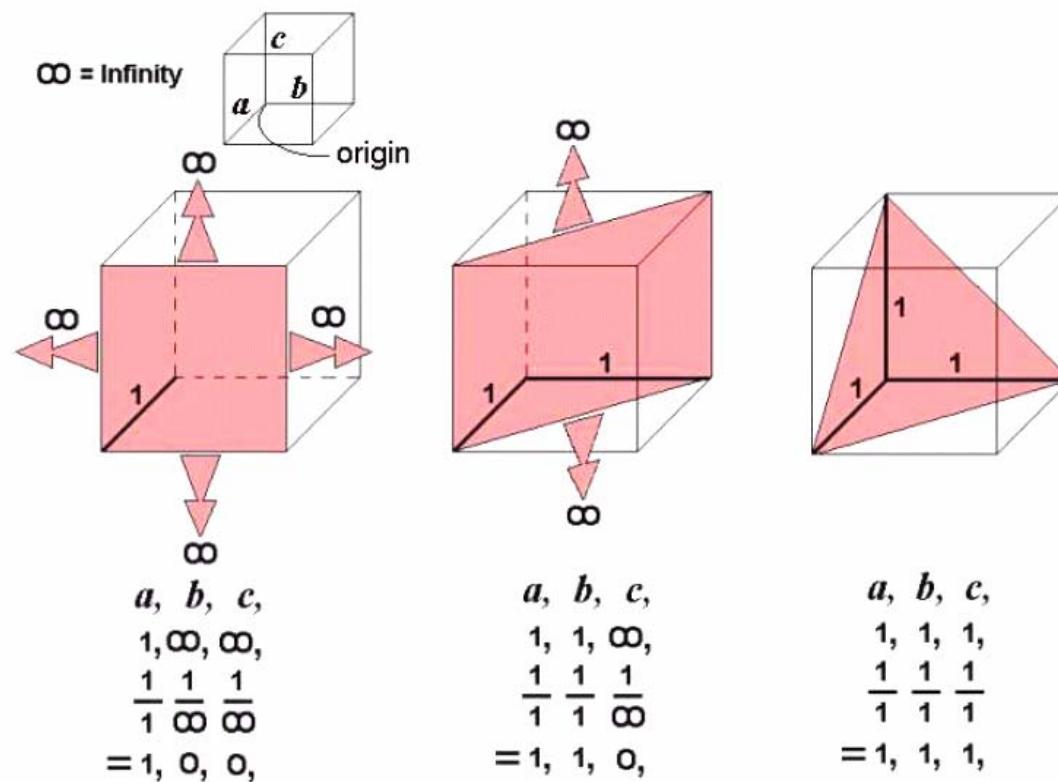
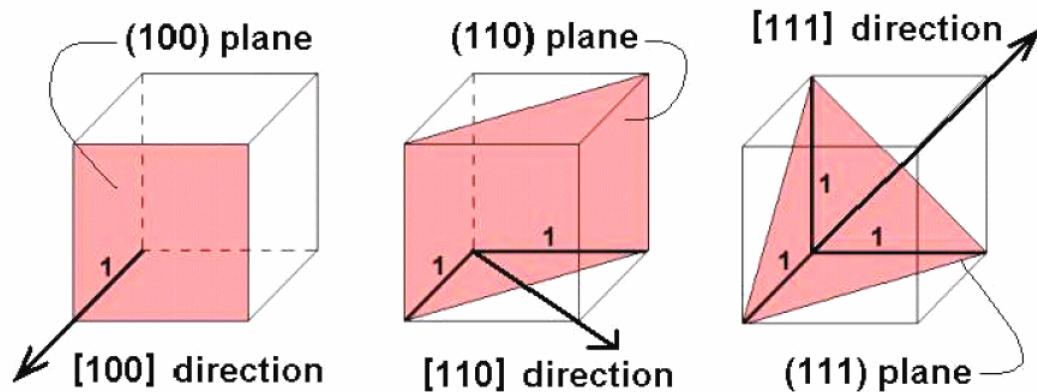
# Miller Indices



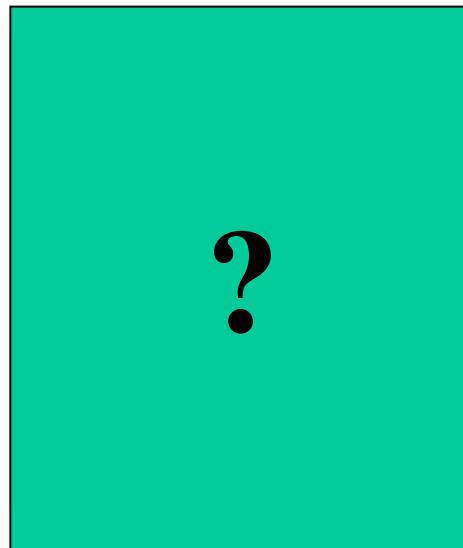
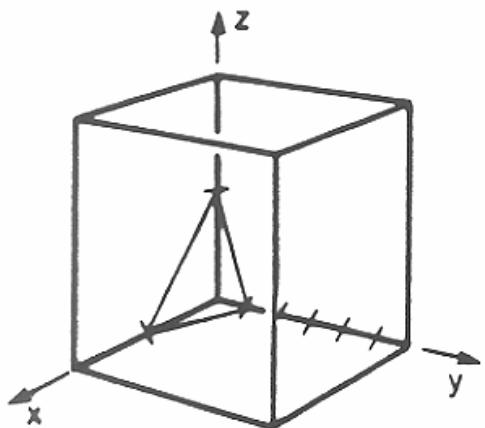


	$x$	$y$	$z$
Intercepts	$\infty$	$\infty$	1
reciprocals	0	0	1
Indices			(001)

## vectors and planes

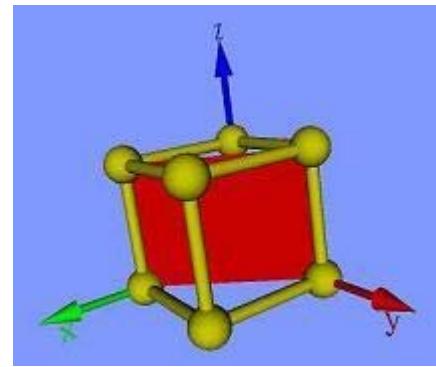


## vectors and planes

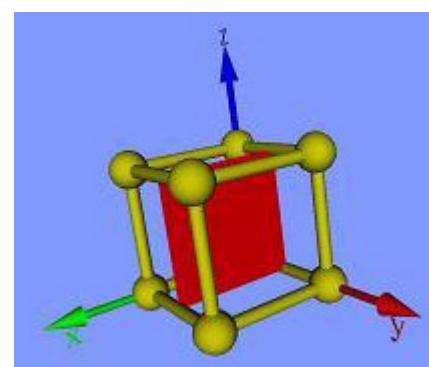


## vectors and planes

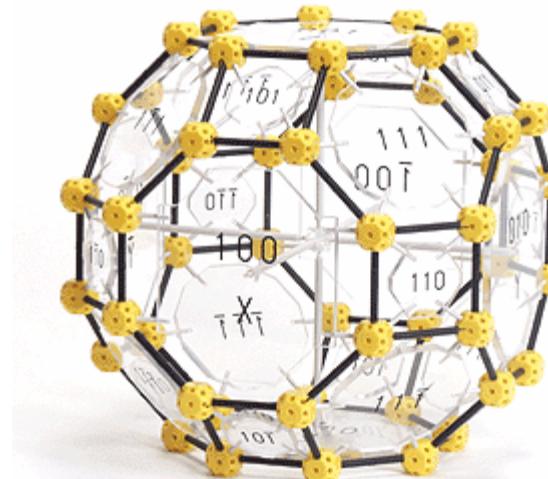
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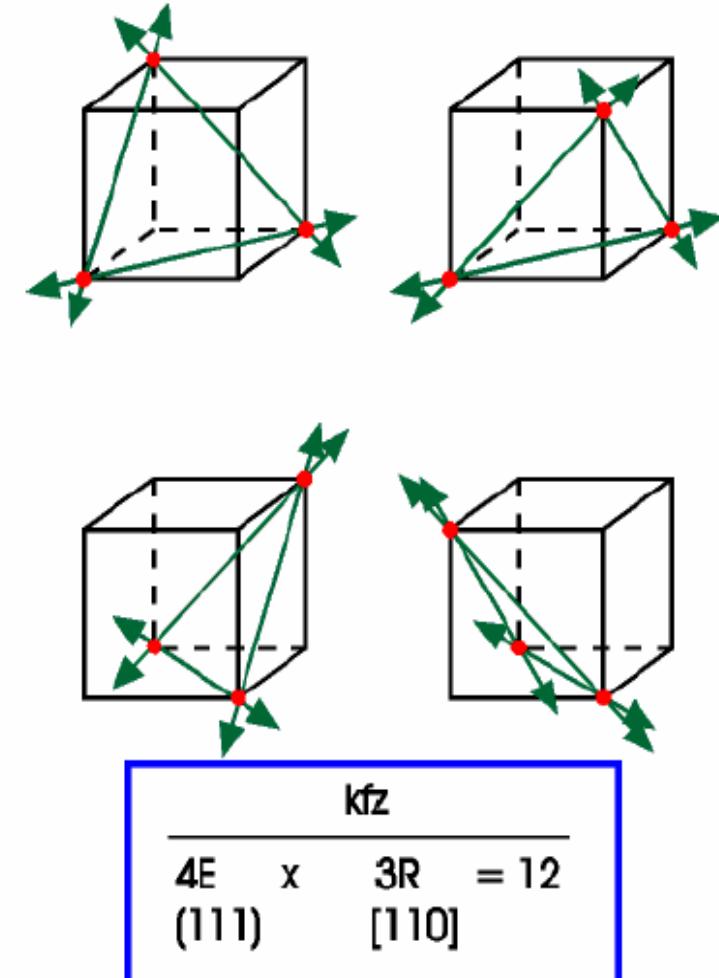
110 plane



020 plane



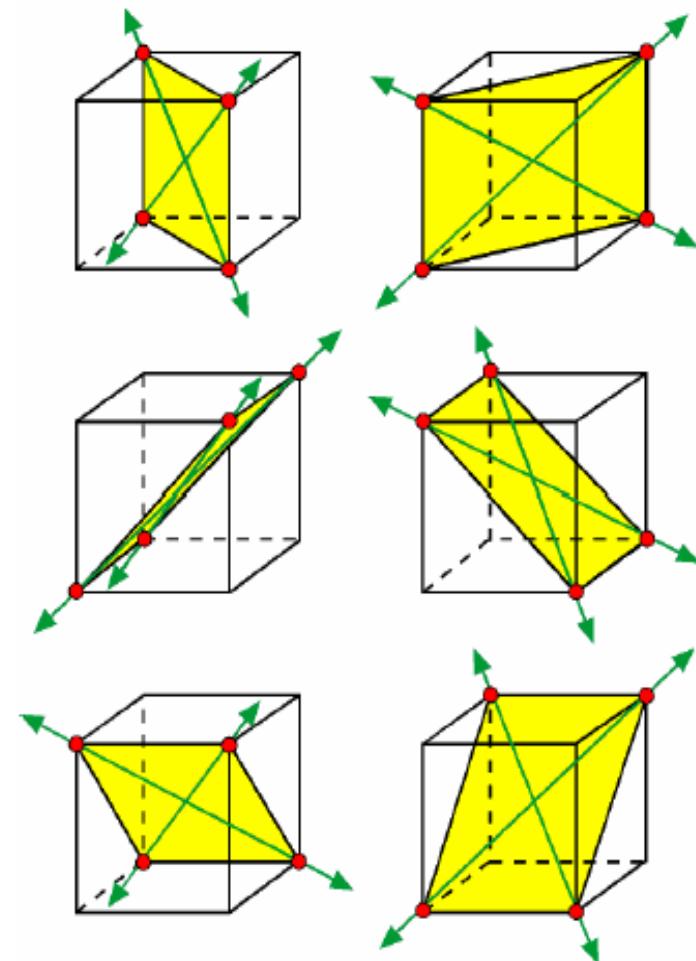
Gittertyp	Basisvektoren $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$	Gleitebenen $G$		Gleitrichtung $\mathbf{g}$		Gesamtzahl der Gleitsysteme
		Typ	Zahl	Typ	Zahl	
k-f-z Al Cu Ni Ag Au		(111)	4	[110]	3	12



## vectors and planes

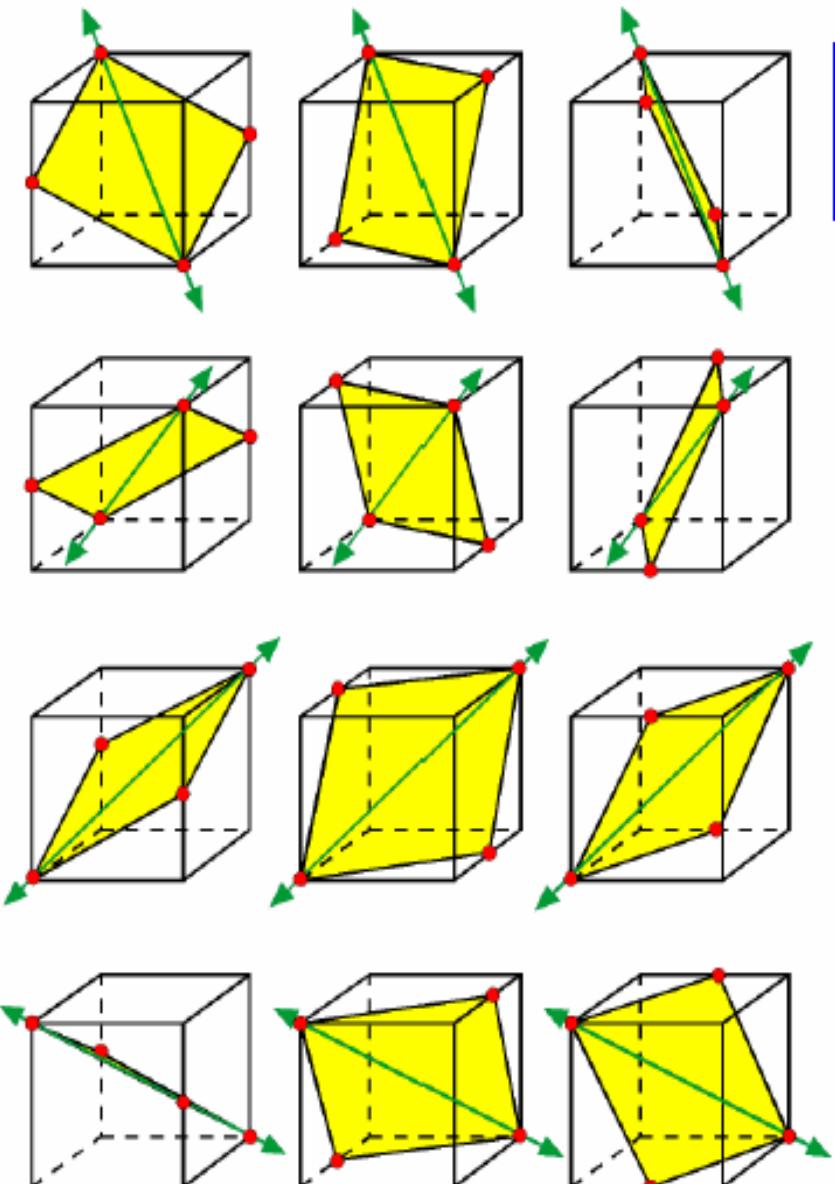
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Gitter typ	Basis einspi- ele		Gleitebe- nen G		Gleitrich- tung g		Gesamt- zahl der Gleitsy- steme
			Typ	Za- h 1	Typ	Za- h 1	
Fe <sub>αδ</sub> W Mo Nb Ta		(110)	6	[111]	2		12
Fe <sub>αδ</sub> W Mo Nb	krz	(112)	12	[111]	1		12
Fe <sub>αδ</sub> W <sub>a</sub> Mo		(123)	24	[111]	1		24

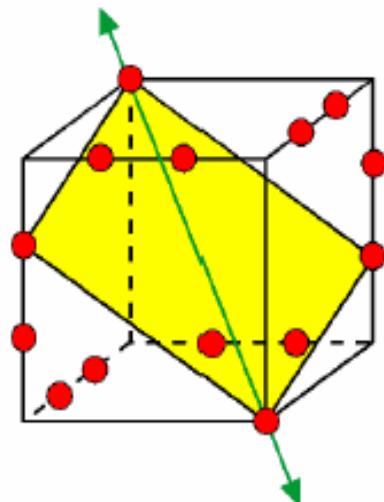


krz		
$6E$	$\times$	$2R = 12$
$(110)$		$[111]$

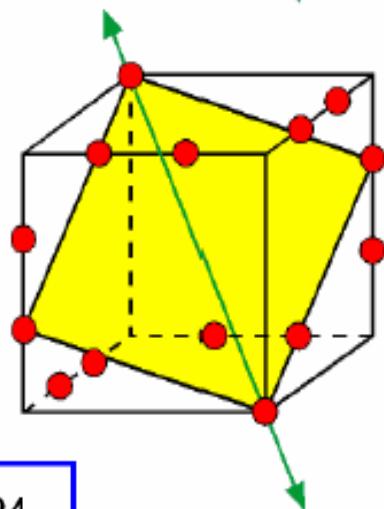
## vectors and planes



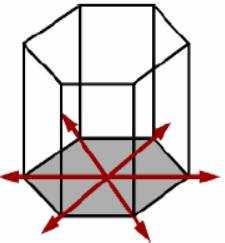
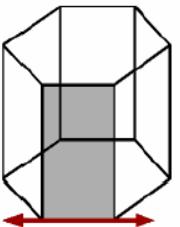
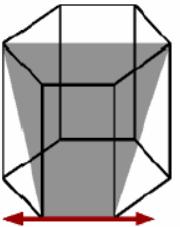
$$12E \times 1R = 12 \\ (112) [111]$$



$$24E \times 1R = 24 \\ (123) [111]$$



## vectors and planes

G i t t e r 1	B e i s p i e l		Gleitebe- nen G		Gleitrich- tung g		Gesamt- zahl der Gleitsy- steme
			Typ	Z a h 1	Typ	Z a h 1	
Cd Zn Mg $Ti_{\alpha}$ Be			(0001)	1	[1120]	3	3
h e x	Cd Zn Mg $Ti_{\alpha}$ Be $Zr_{\alpha}$		(1010)	3	[1120]	1	3
Mg $Ti_{\alpha}$			(1011)	6	[1120]	1	6

## vectors and planes

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

$$<110> = [1,1,0] \begin{bmatrix} \bar{1},1,0 \\ 1,\bar{1},0 \\ \bar{1},\bar{1},0 \\ 1,0,1 \\ \bar{1},0,\bar{1} \end{bmatrix} \dots$$

specific

general

direction

[ ]

< >

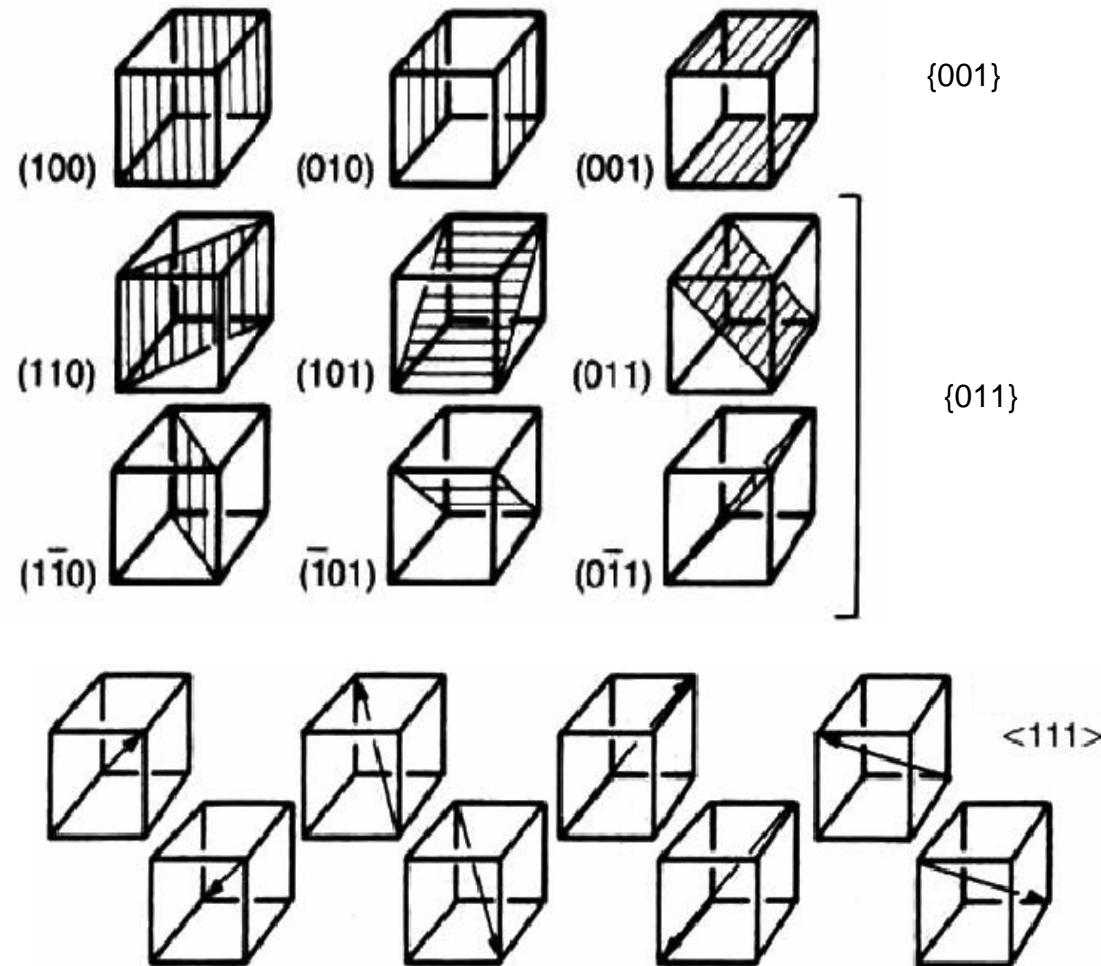
plane

( )

{ }

## vectors and planes

# family of lattice planes



## vectors and planes

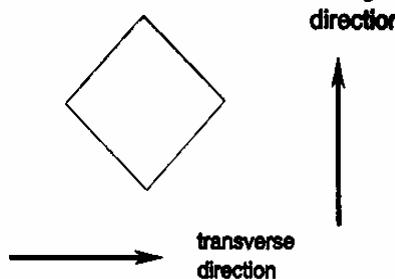
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## Miller Indices for 3D orientations

$\{hkl\} <uvw>$

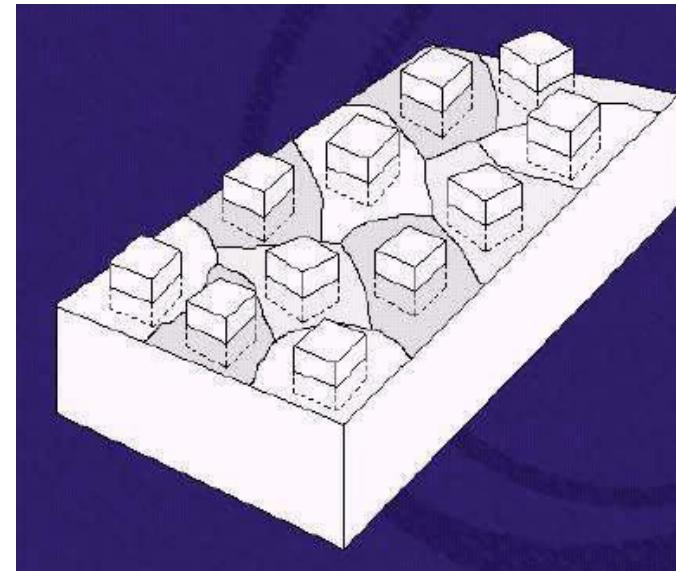
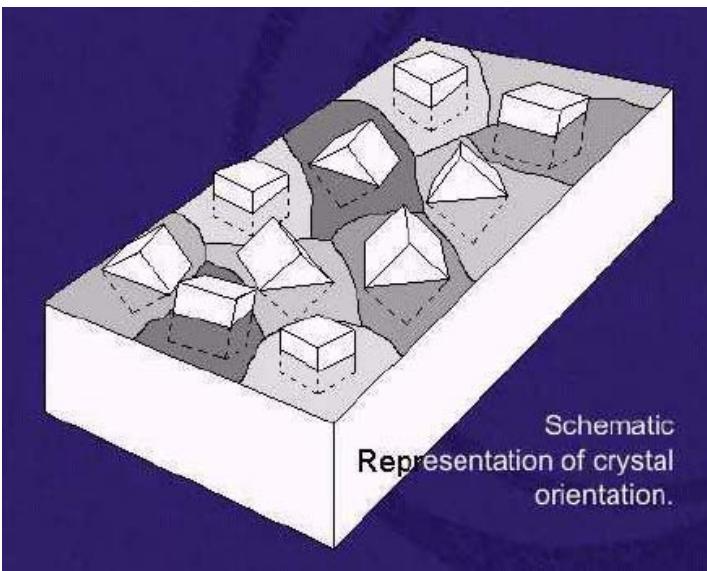
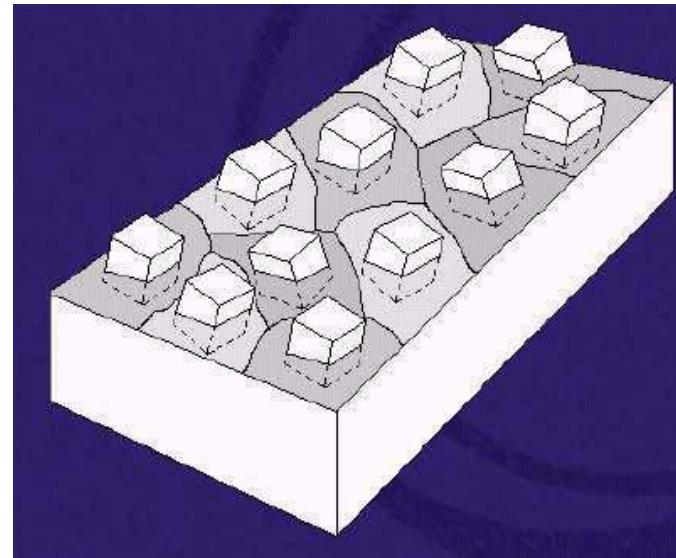
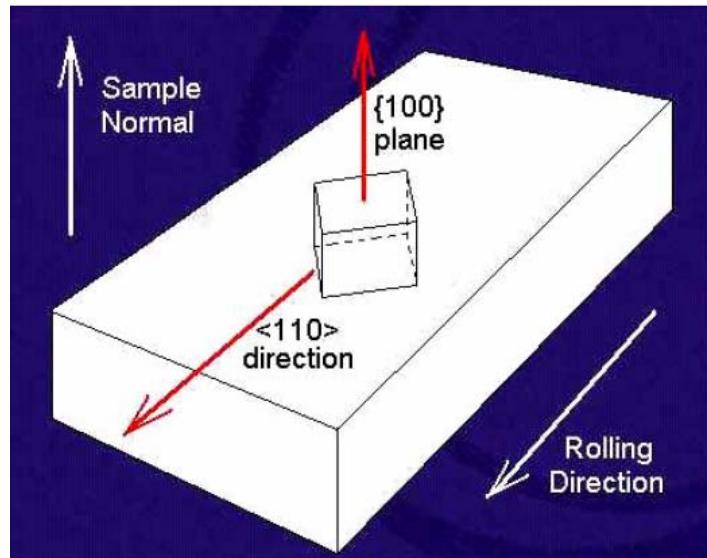
$\{001\} <110>$

$\varphi_1 \Phi \varphi_2$



## Texture, Miller-Indices

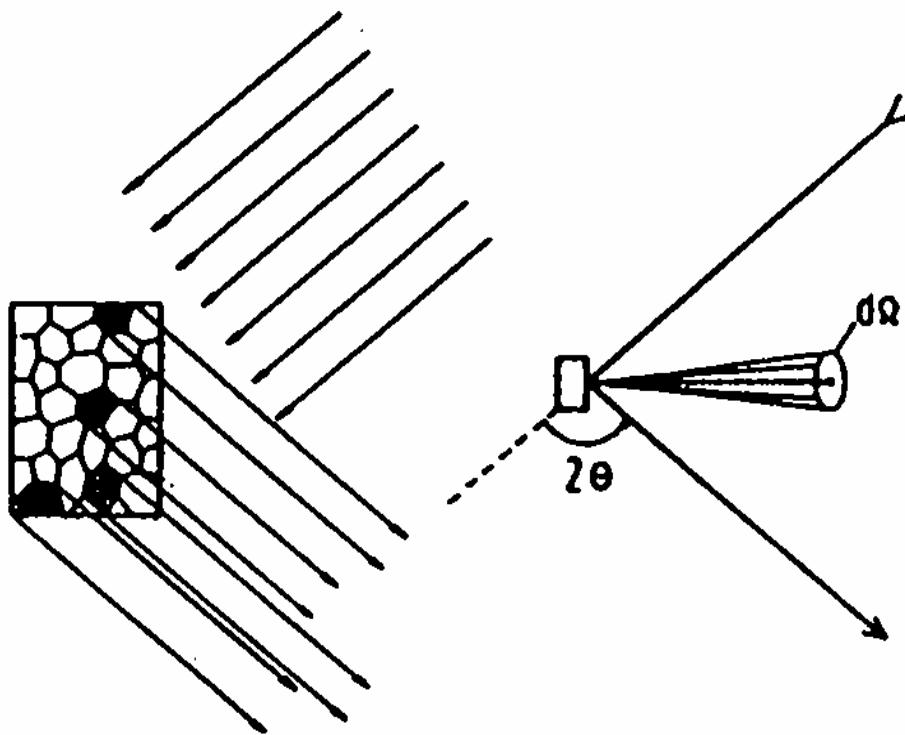
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## Texture, Miller-Indices

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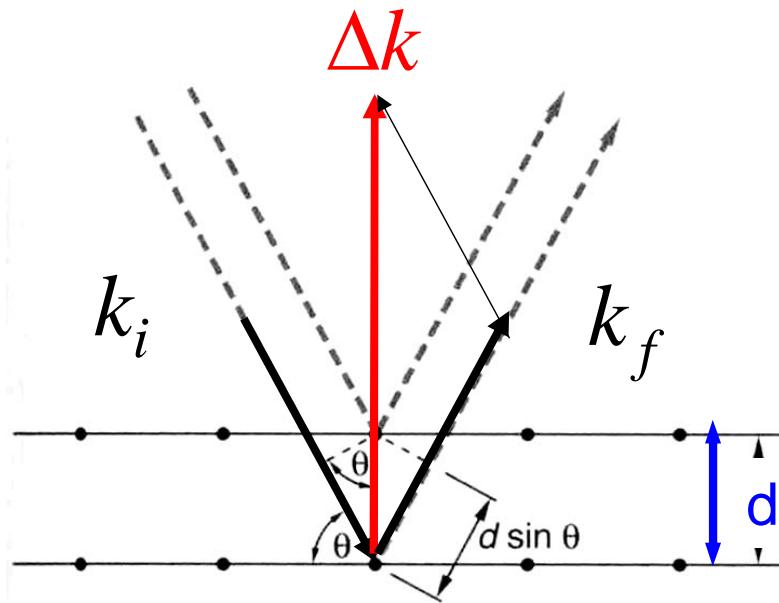
$$n \lambda = 2 d \sin \Theta$$



## Bragg Equation

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## Bragg's Law



$$n\lambda = 2d_{hkl} \sin \theta$$

$$\text{where } k = \frac{2\pi}{\lambda}$$

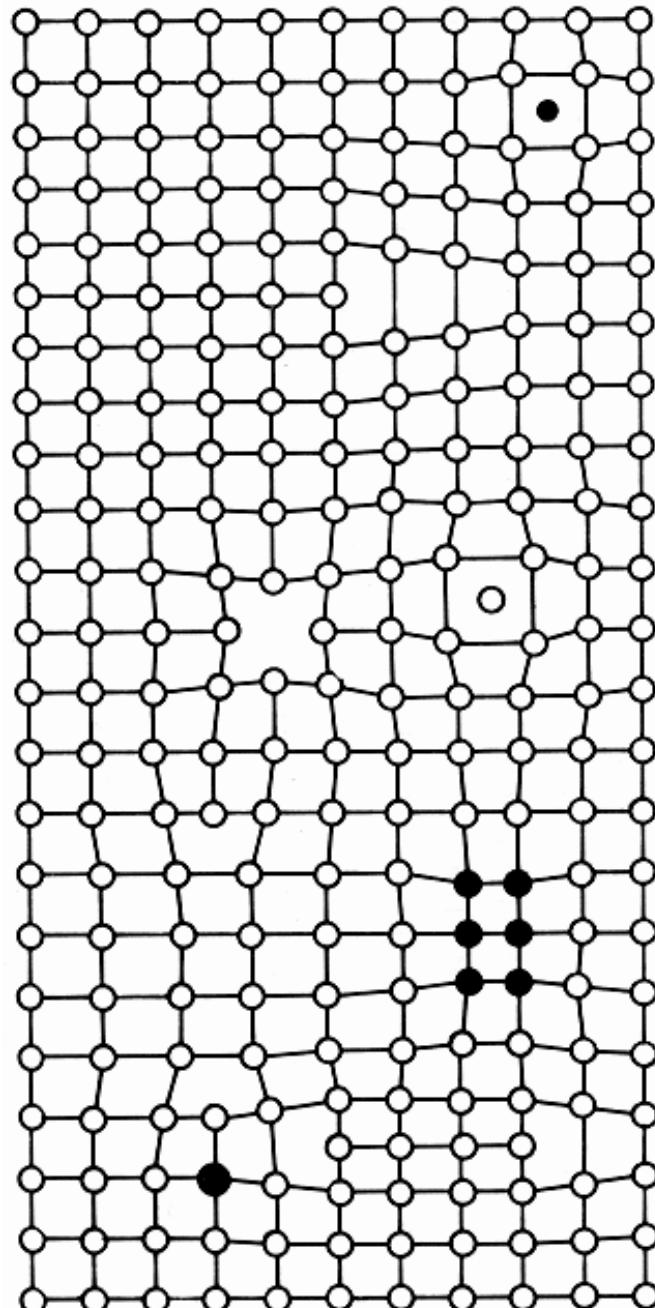


# Dislocation mechanics

- crystal defects : - point defects
  - dislocations
  - grain and phase boundaries
- dislocations:
  - evidence
  - types
- mechanisms of plastic deformation
  - crystallographic slip
  - Schmid's law
  - elastic properties of dislocations
  - interaction of dislocations and origin

# Crystal defects

- zero dimensional point defects: vacancies and insterstitials
- one-dimensional line defects: disloactions
- two-dimensional planar defects: grain and phase boundaries
- three-dimensional defects: different phases



- interstitial atom
- edge dislocation
- self interstitial atom
- vacancy
- precipitate of impurity atoms
- vacancy type dislocation loop
- interstitial type dislocation loop
- substitutional atom

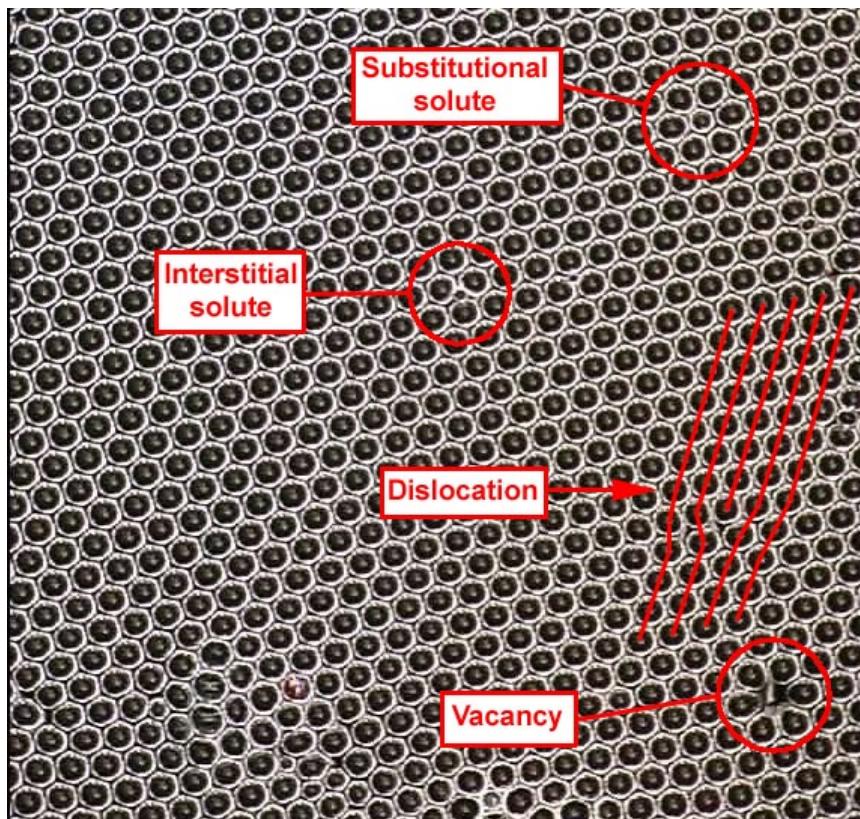
# Existence of defects

The concept of the dislocation was invented independently by Orowan, Taylor and Polanyi in 1934 as a way of explaining two key observations about the plastic deformation of crystalline material:

- The stress required to plastically deform a crystal is much less than the stress one calculates from considering a defect-free crystal structure
- Materials work-harden: when a material has been plastically deformed it subsequently requires a greater stress to deform further.

Not until 1947 was the existence of dislocations experimentally verified. It took another ten years before electron microscopy techniques were advanced enough to show dislocations moving through a material.

# Types of dislocations

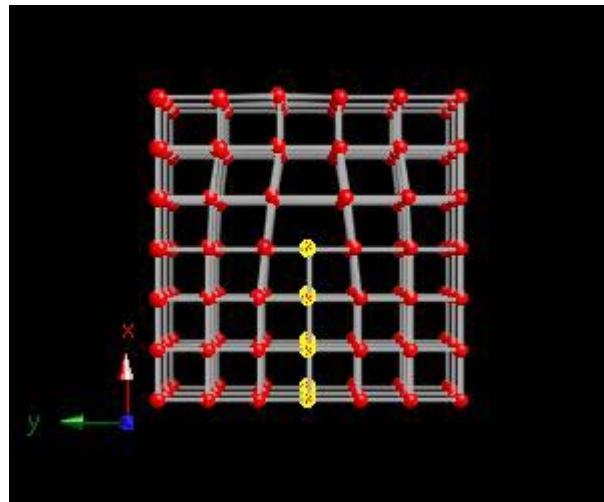


A dislocation in a 2D close-packed plane can be described as an extra 'half-row' of atoms in the structure. Dislocations can be characterised by the Burgers vector which gives information about the orientation and magnitude of the dislocation.

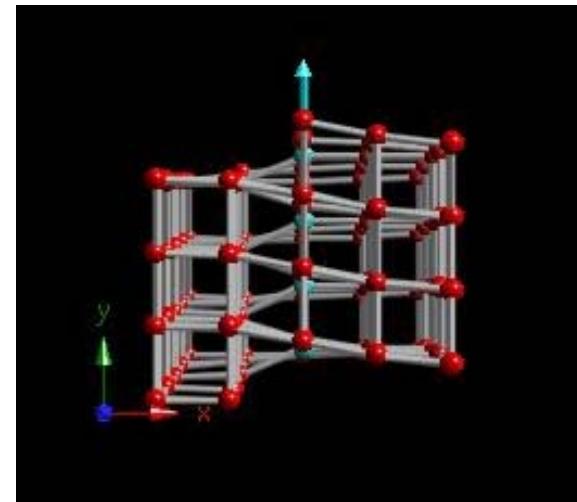
Bubble raft

# Types of dislocations

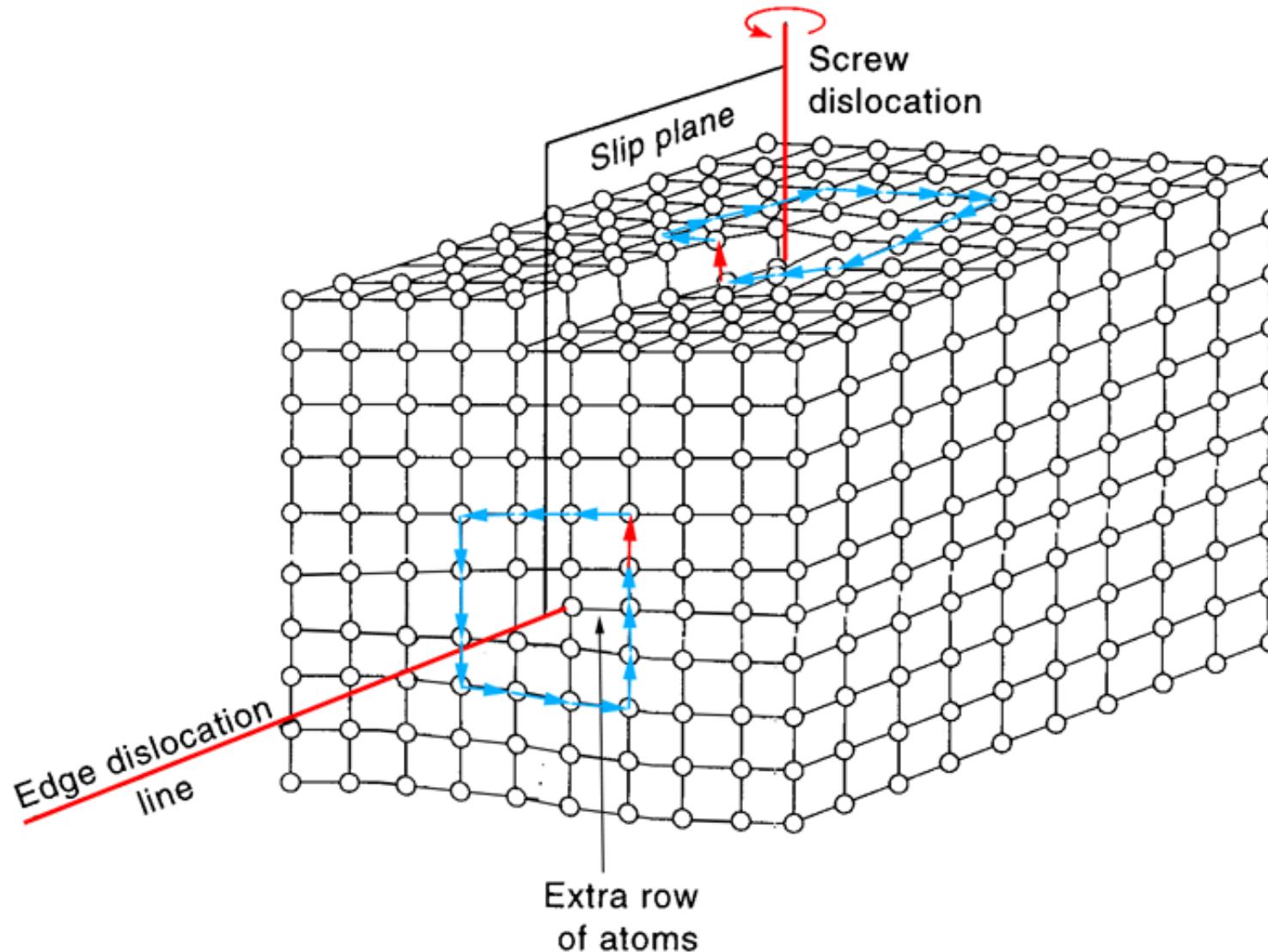
edge dislocation



screw dislocation

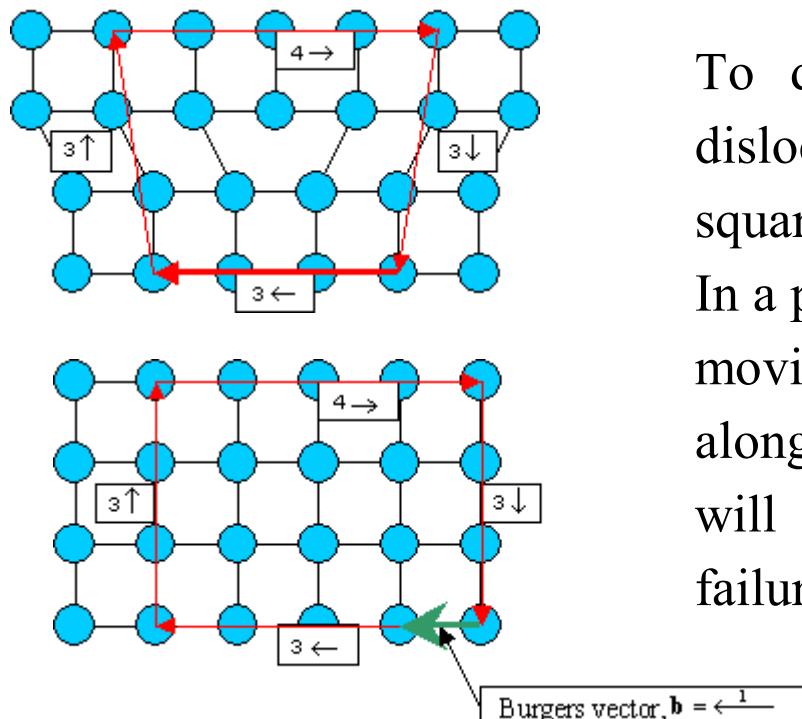


# Types of dislocations



# The Burgers vector

The Burgers vector of a dislocation is a crystal vector, specified by Miller indices, that quantifies the difference between the distorted lattice around the dislocation and the perfect lattice. Equivalently, the Burgers vector denotes the direction and magnitude of the atomic displacement that occurs when a dislocation moves.

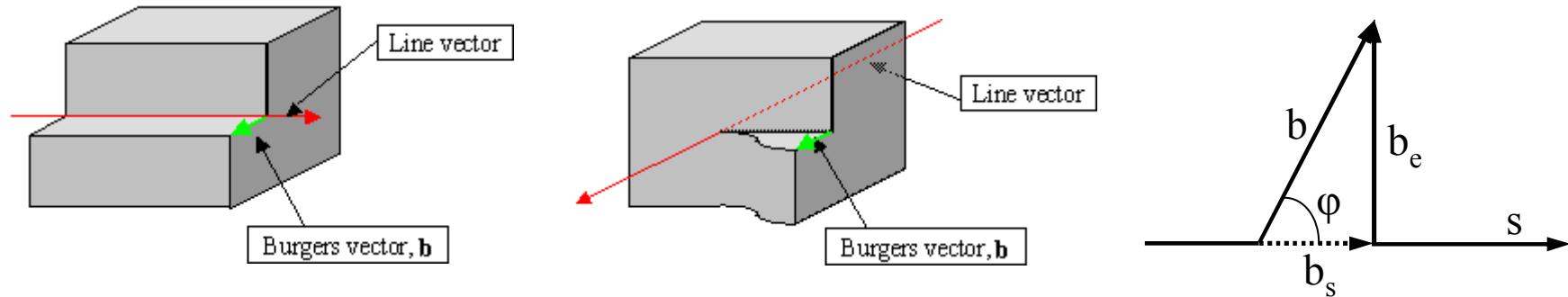


To determine the Burgers vector of a dislocation in a two-dimensional primitive square lattice, proceed as follows:

In a perfect lattice, trace out the same path, moving the same number of lattice vectors along each direction as before. This loop will not be complete, and the closure failure is the Burgers vector:

$$\text{Burgers vector, } \mathbf{b} = \leftarrow \frac{1}{\square}$$

An edge dislocation has its Burgers vector perpendicular to the dislocation line. Edge dislocations are easiest to visualise as an extra half-plane of atoms. A screw dislocation is more complex - the Burgers vector is parallel to the dislocation line. Mixed dislocations also exist, where the Burgers vector is at some acute angle to the dislocation line.



When a dislocation moves under an applied shear stress:

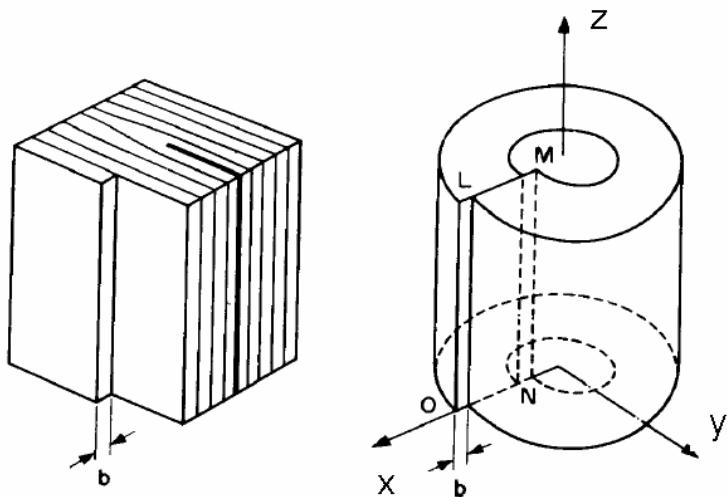
- individual atoms move in directions parallel to the Burgers vector
- the dislocation moves in a direction perpendicular to the dislocation line

An edge dislocation therefore moves in the direction of the Burgers vector, whereas a screw dislocation moves in a direction perpendicular to the Burgers vector. The screw dislocation 'unzips' the lattice as it moves through it, creating a 'screw' or helical arrangement of atoms around the core.

dislocation loop

prismatic dislocation loop

## Stress field of straight edge dislocation



"Recipe" :

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

Situation is *plane-strain*. No displacements in z-direction.

Derivation of stress tensor is complicated.

(see Hirth and Lothe for the full works)

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

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

$$\sigma_{yy} = Dy \frac{x^2 - y^2}{(x^2 + y^2)^2}$$

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

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

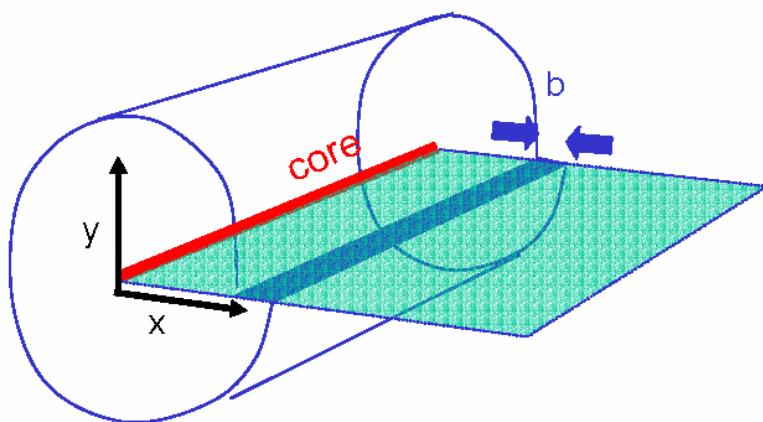
Hydrostatic Stress, P:

$$P = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = \frac{2(1+\nu)}{3}D \frac{y}{x^2 + y^2}$$

Note:

- Stress and strain fields are *not* pure shear
- Stresses and strains are proportional to  $1/r$ :
  - extend to infinity
  - tend to infinite values as  $r \rightarrow 0$

## Strain energy of an edge dislocation



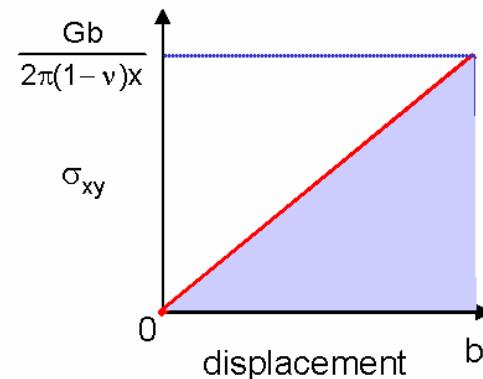
with dislocation in place,

$$\sigma_{xy} = \sigma_{yx} = \frac{Gb}{2\pi(1-\nu)} x \frac{x^2 - y^2}{(x^2 + y^2)^2}$$

at  $y = 0$ :

$$\sigma_{xy} = \frac{Gb}{2\pi(1-\nu)x}$$

Now imagine *making* the dislocation by cutting on green plane and displacing the two sides by relative  $b$



Work done at  $x$

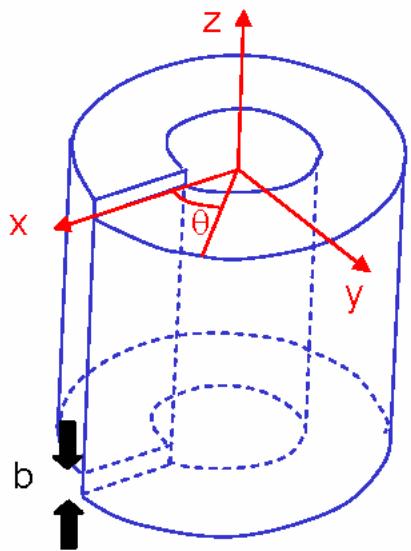
$$= \frac{1}{2} \frac{Gb}{2\pi(1-\nu)x} b$$

Total work done between  $r_0$  and  $R$

$$= \int_{r_0}^R \frac{Gb^2}{4\pi(1-\nu)x} dx \\ = \frac{Gb^2}{4\pi(1-\nu)} \ln\left(\frac{R}{r_0}\right)$$

This must equal the elastic energy per unit length of the dislocation.

# Strain field of 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:  $u_x = u_y = 0$

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

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

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

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

## Stress field of straight screw dislocation

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

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

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



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

$$\Delta = 0$$

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

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

In Polar coordinates:

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

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

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

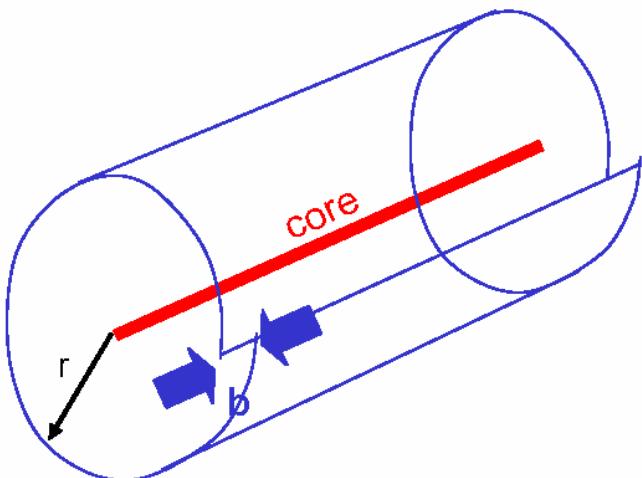
All other components of the stress tensor are zero.

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  $r_0 \approx 1 \text{ nm}$ .

## Strain energy of a screw dislocation



In the shell shown,

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

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

All other stresses and strains are zero.

Elastic energy per unit volume =

$$\frac{1}{2}(\varepsilon_{\theta z}\sigma_{\theta z} + \varepsilon_{z\theta}\sigma_{z\theta}) = \frac{Gb^2}{8\pi r^2}$$

Volume of shell, thickness  $\delta r = 2\pi r \cdot \delta r$

Elastic energy of shell =

$$\frac{Gb^2}{4\pi r} \delta r$$

Total elastic energy

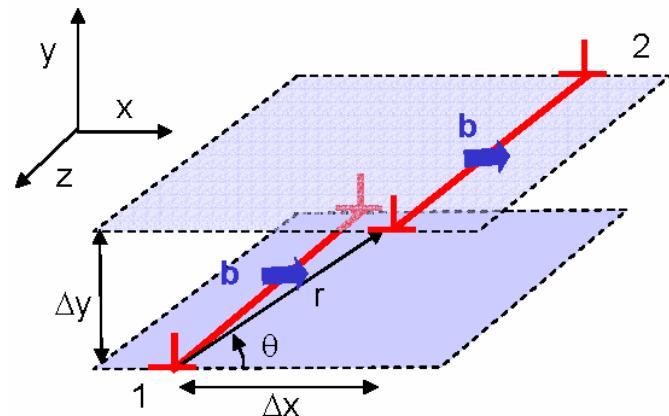
$$= \int_{r_0}^R \frac{Gb^2}{4\pi r} dr$$

$$= \frac{Gb^2}{4\pi} \ln\left(\frac{R}{r_0}\right)$$

per unit length of  
dislocation line

## dislocations

## Forces between edge dislocations



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

The important components of the stress field are:

$\sigma_{xy}$  – produces *glide* force on disln 2;

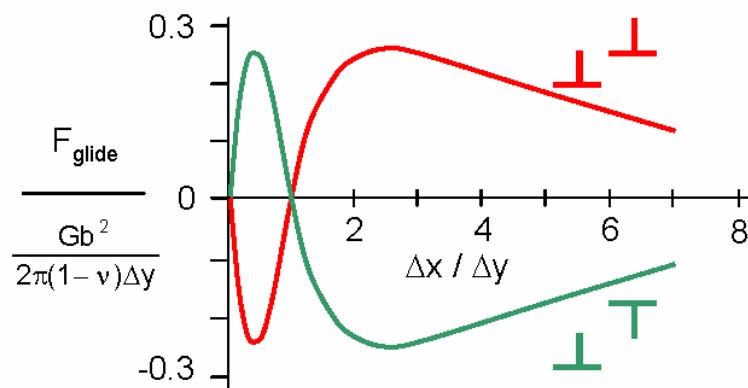
$\sigma_{xx}$  – produces *climb* force on disln 2.

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

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

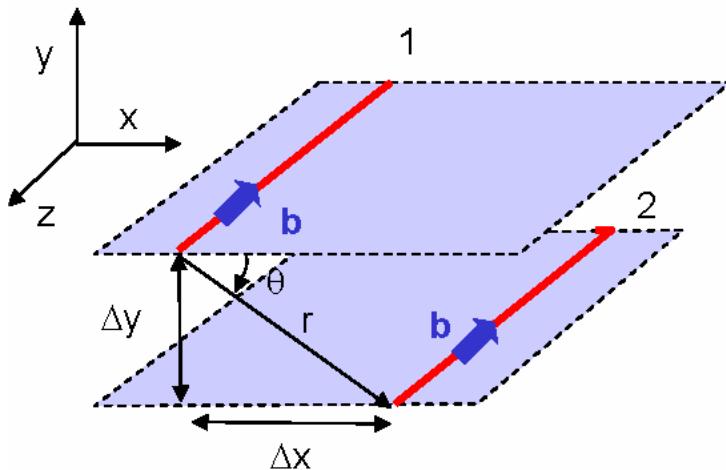
So glide force, resolved onto the slip plane, is:

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



## dislocations

## Forces between 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:

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

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

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

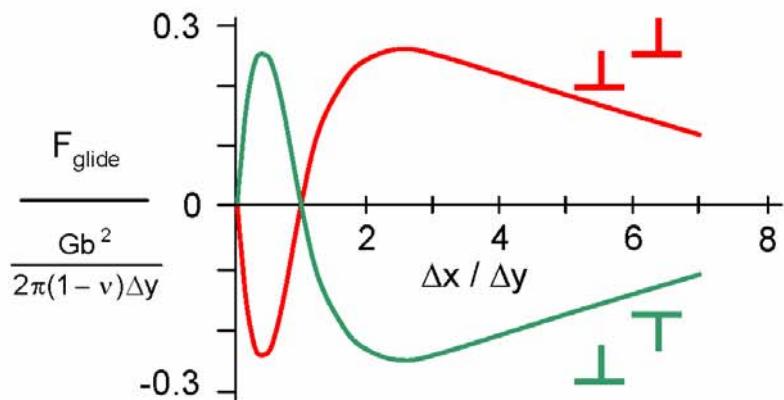
$$\sigma_{xz} = -\frac{Gb}{2\pi} \frac{\Delta y}{\Delta x^2 + \Delta y^2} = -\frac{Gb \sin\theta}{2\pi r}$$

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

Note that the shear stress acting to shear atoms parallel to **b** above and below the glide plane is  $\sigma_{yz}$ .

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

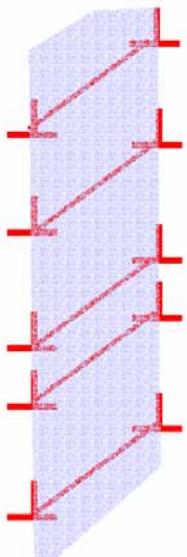
## Stable arrangements for edge dislocations



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

A low angle tilt boundary.

This arrangement has a strong long-range stress field.

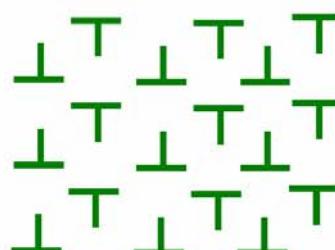


For **like** Burgers vectors:  
 $\Delta x = \pm \Delta y$ : unstable equilibrium  
 $\Delta x = 0$  : stable equilibrium

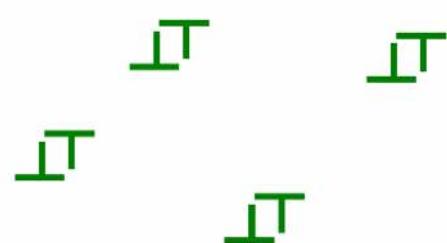
For **opposite** Burgers vectors:  
 $\Delta x = \pm \Delta y$ : stable equilibrium  
 $\Delta x = 0$  : unstable equilibrium

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

There are a large number of possible stable arrangements.



"Taylor lattice"



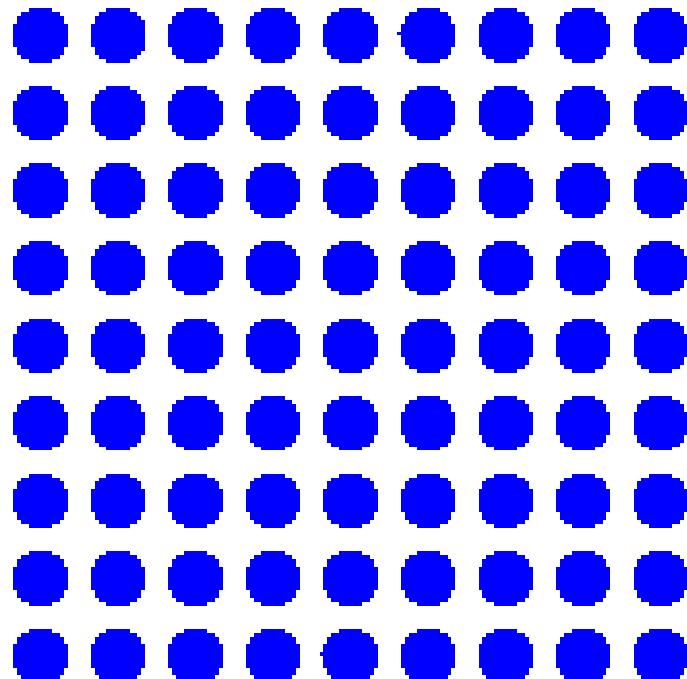
"Dipole dispersion"

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

## dislocations

dislocation: multiplication + motion → deformation

slip planes

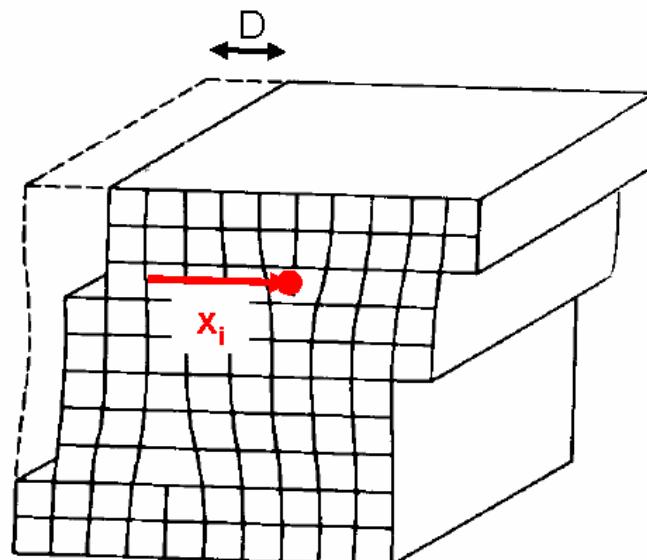
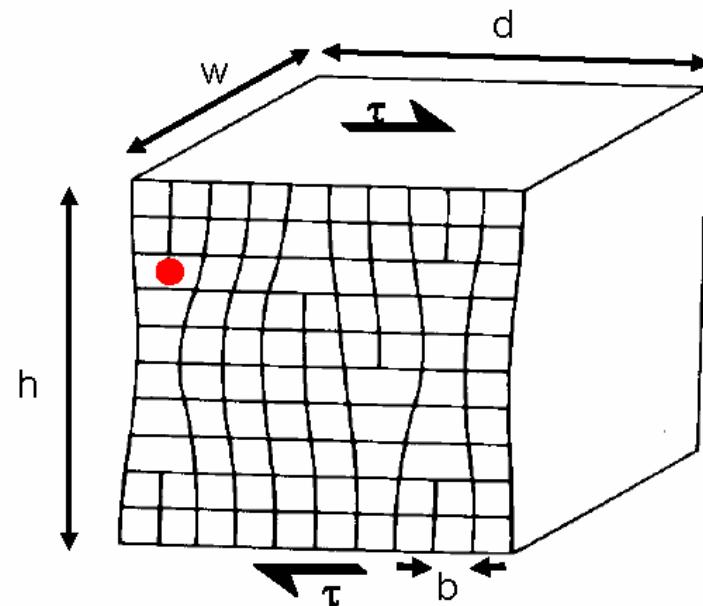


1 dislocation

**dislocations**

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# Strain rate from motion of dislocations



If a dislocation moved the whole length of the crystal  $d$ , it would contribute  $\mathbf{b}$  to the displacement  $\mathbf{D}$ .

If each dislocation moves an amount  $x_i$  (less than  $d$ ), then each will contribute  $(x_i / d) \cdot \mathbf{b}$  to  $\mathbf{D}$ .

$$D = \frac{b}{d} \sum_i x_i$$

Shear strain is:

$$\varepsilon = \frac{D}{h} = \frac{b}{dh} \sum_i x_i$$

Define average distance moved by each dislocation:

$$\bar{x} = \frac{1}{N} \sum_i x_i$$

Density of *mobile* dislocations is:

$$\rho_m = \frac{N}{hd}$$

Strain rate:

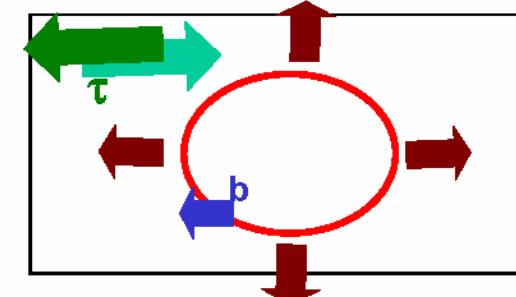
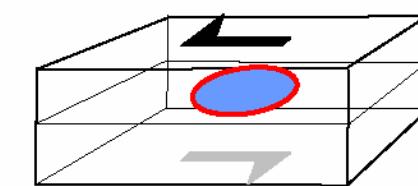
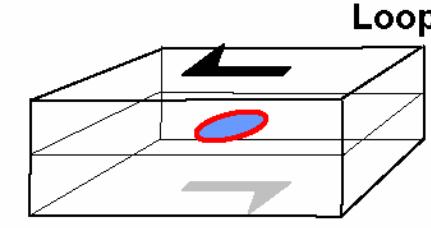
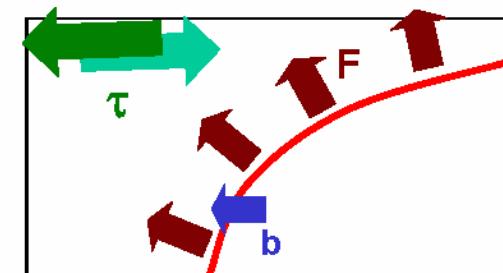
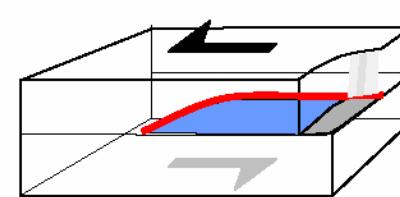
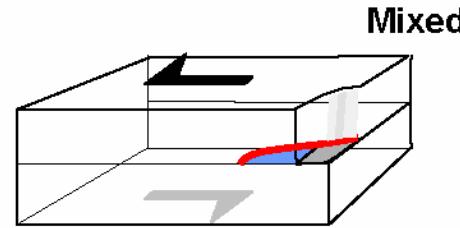
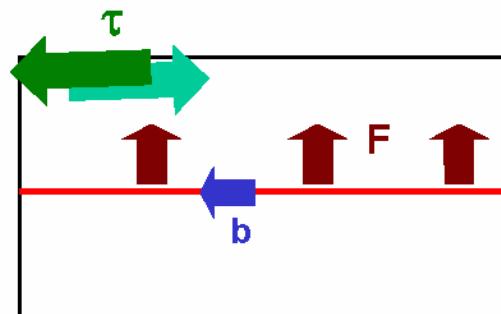
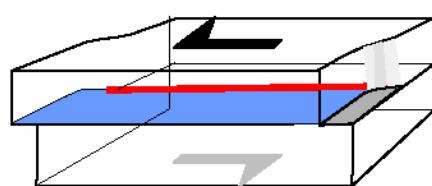
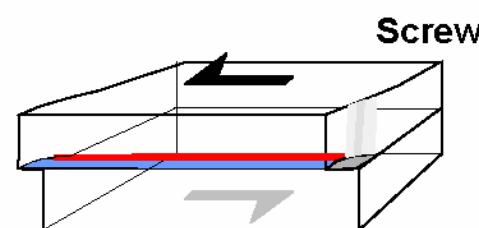
$$\dot{\varepsilon} = \boxed{\frac{d\varepsilon}{dt}} = b\rho_m \frac{d\bar{x}}{dt} = \boxed{b\rho_m \bar{v}}$$

- where  $\bar{v}$  is the average dislocation glide velocity.

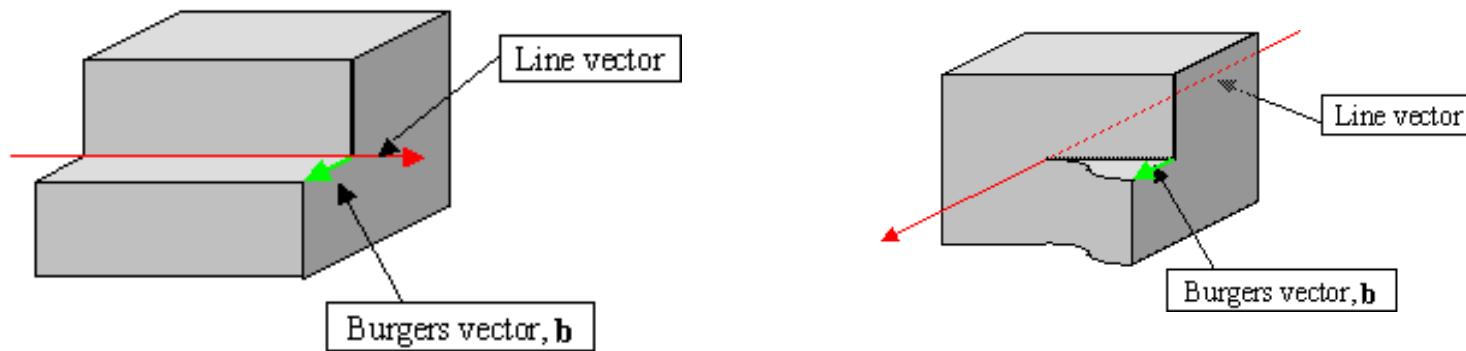
# Forces on dislocations

Dislocation motion only has "meaning" normal to the line vector.

Forces on dislocations can only act normal to the line vector.



## dislocations



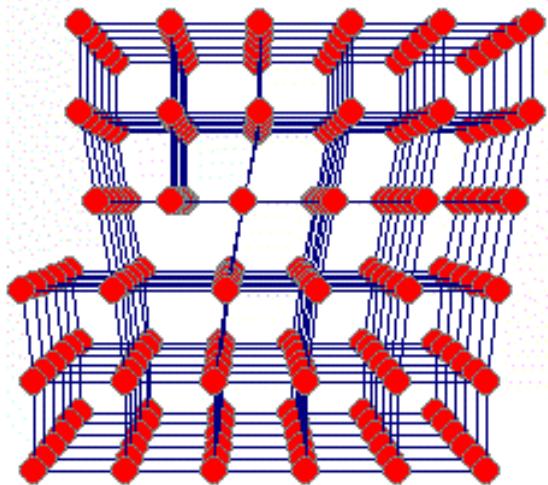
## dislocations

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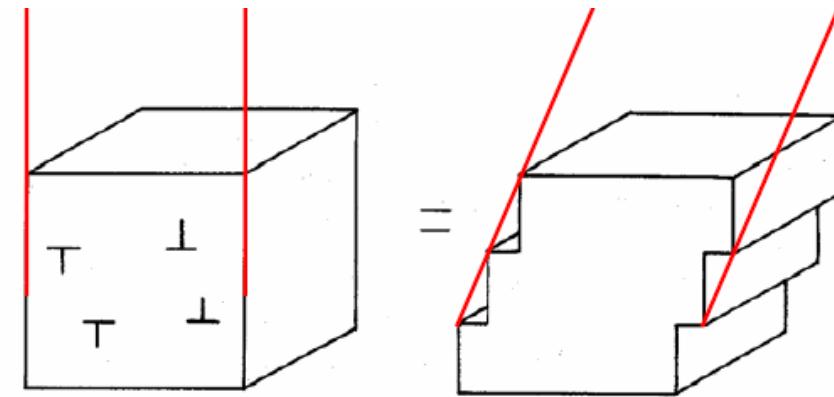
# **hier weitermachen**

dislocation: multiplication + motion → deformation

1 dislocation

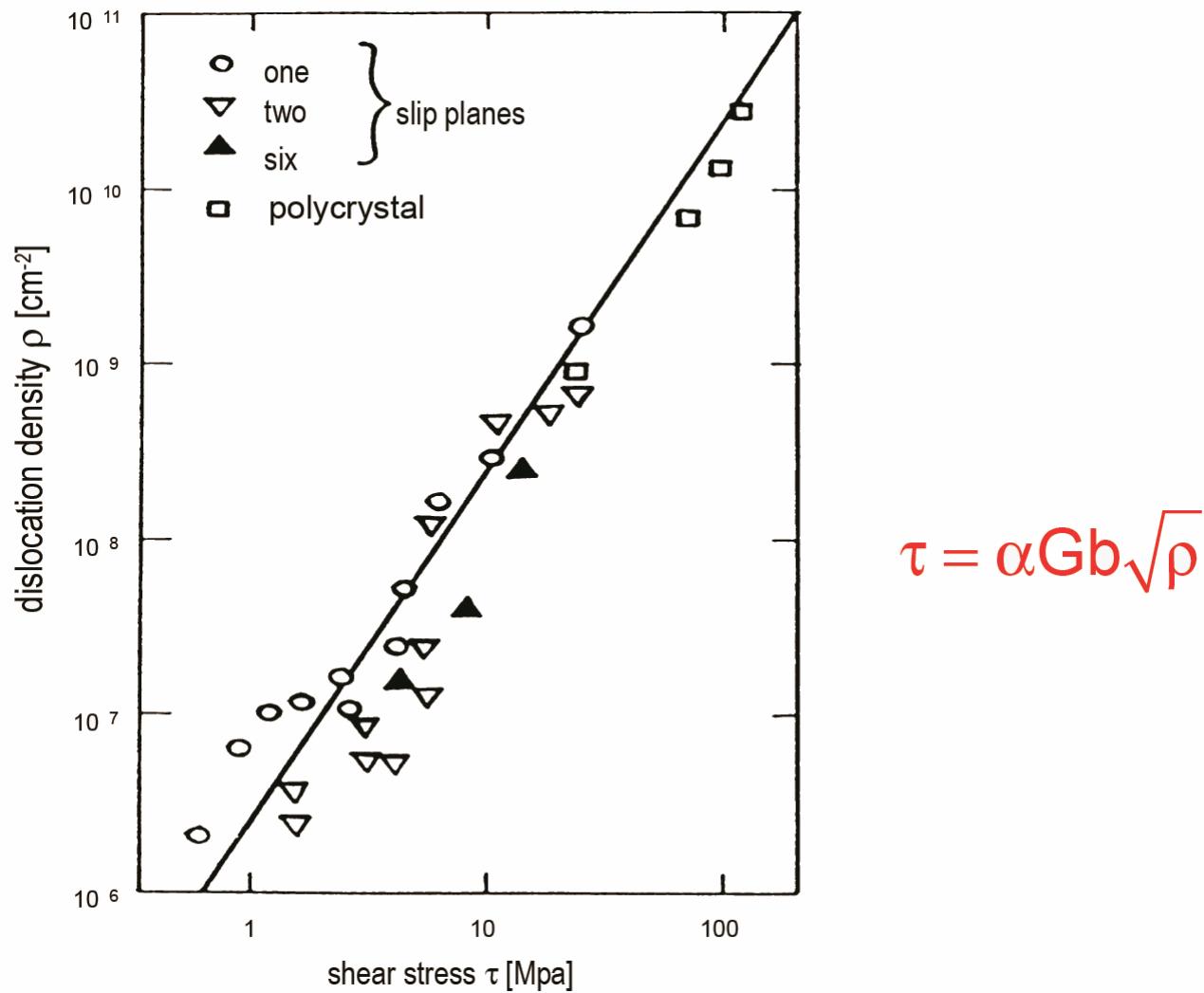


many dislocations

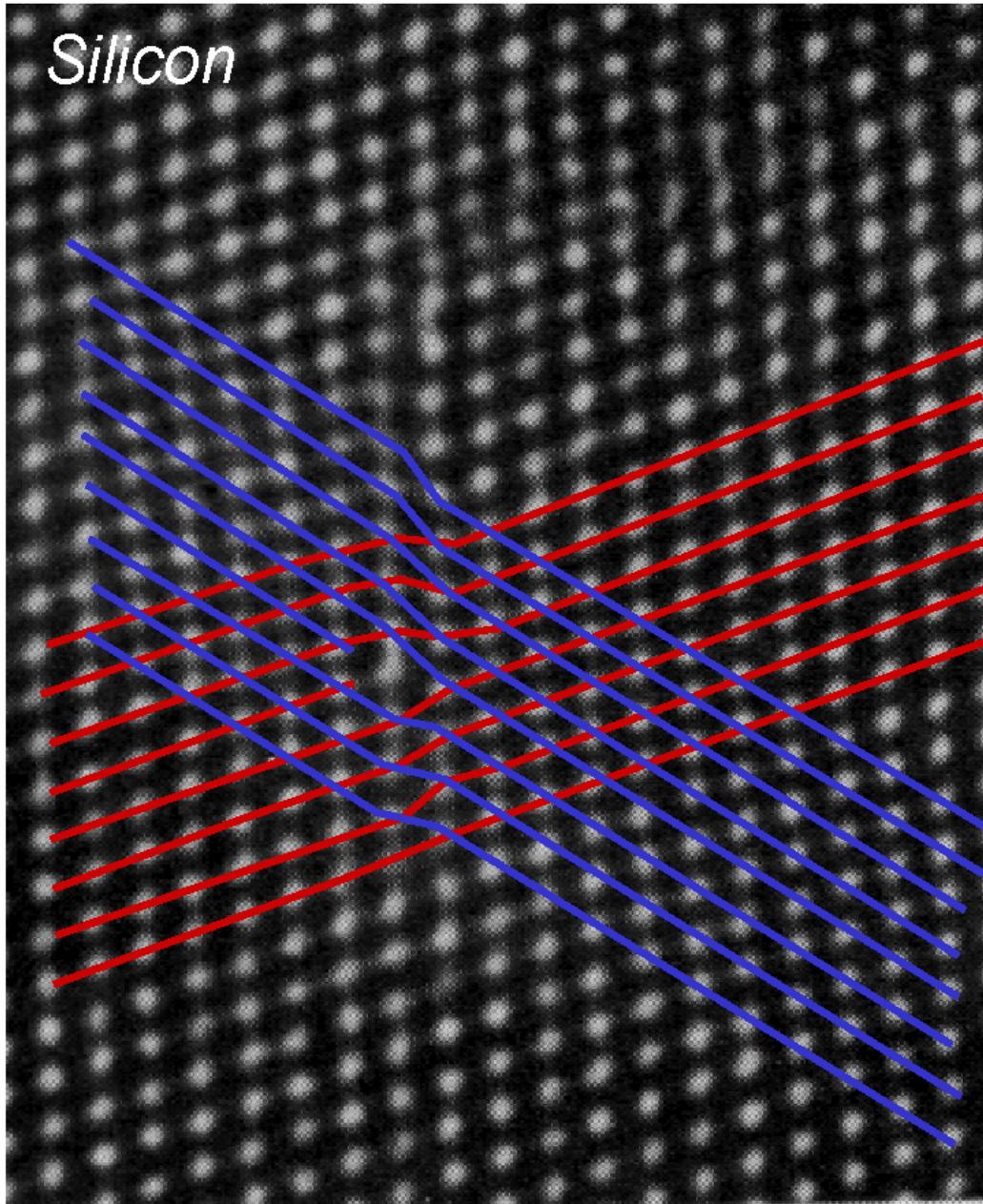


**dislocations**

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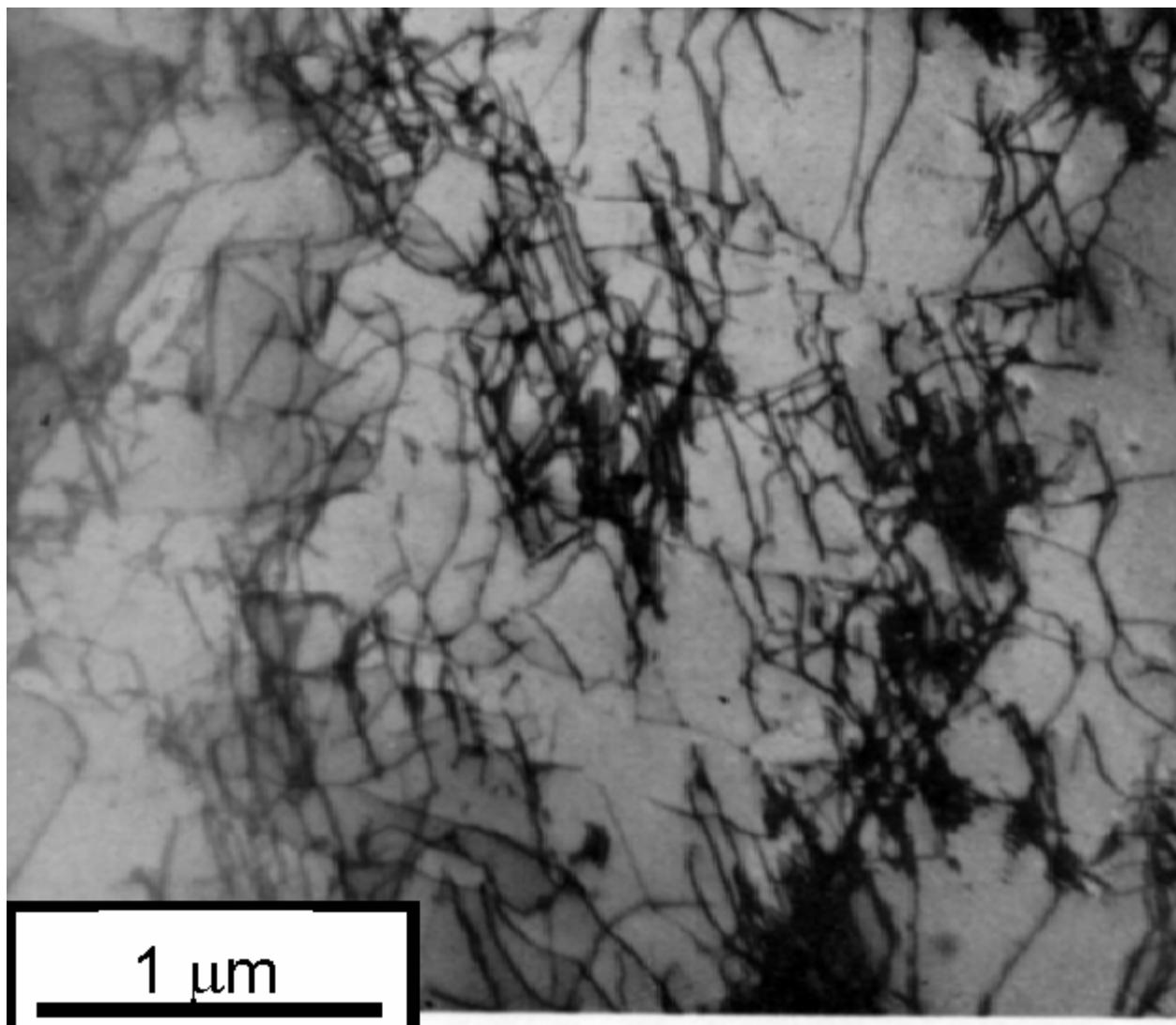


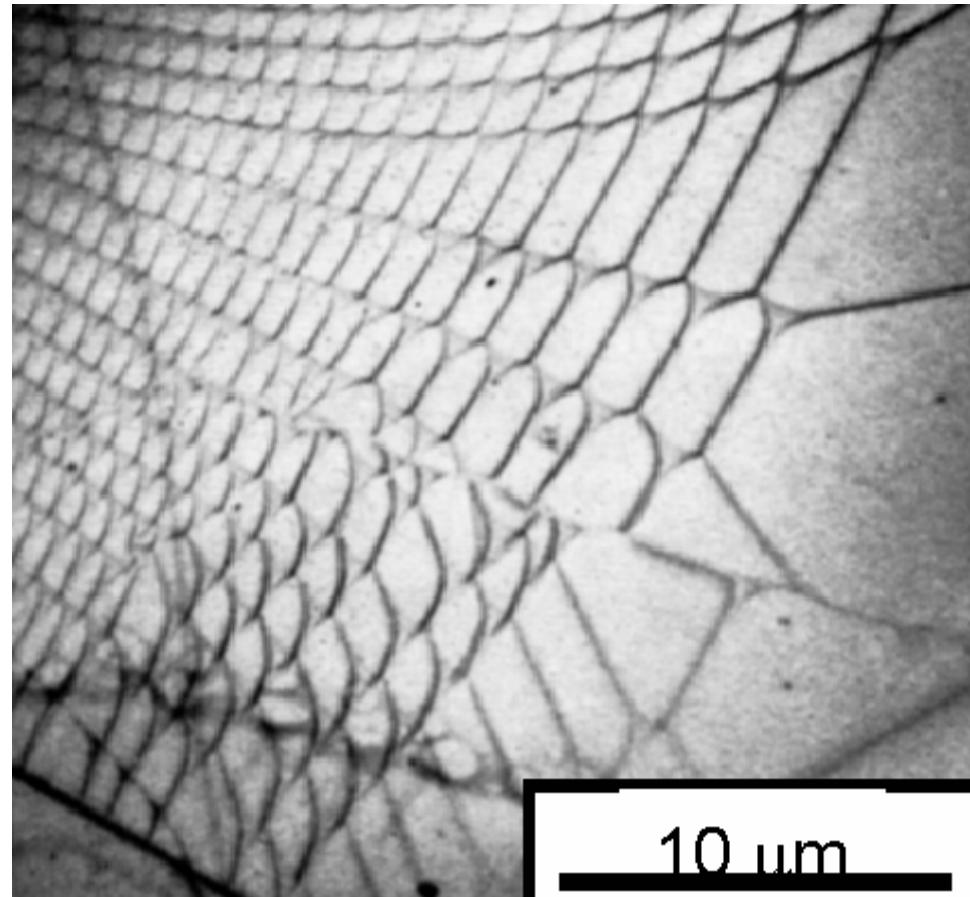
*Silicon*

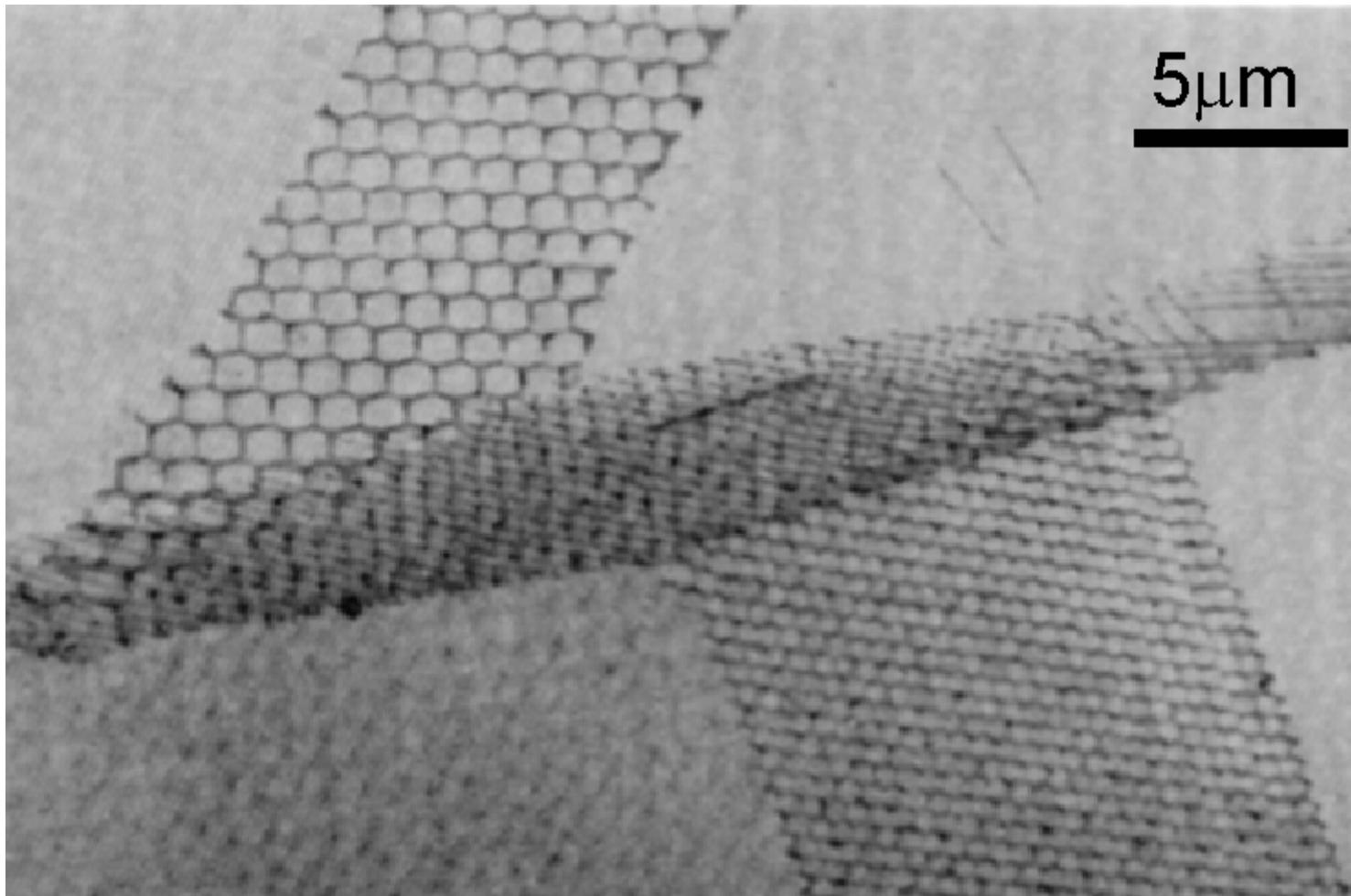


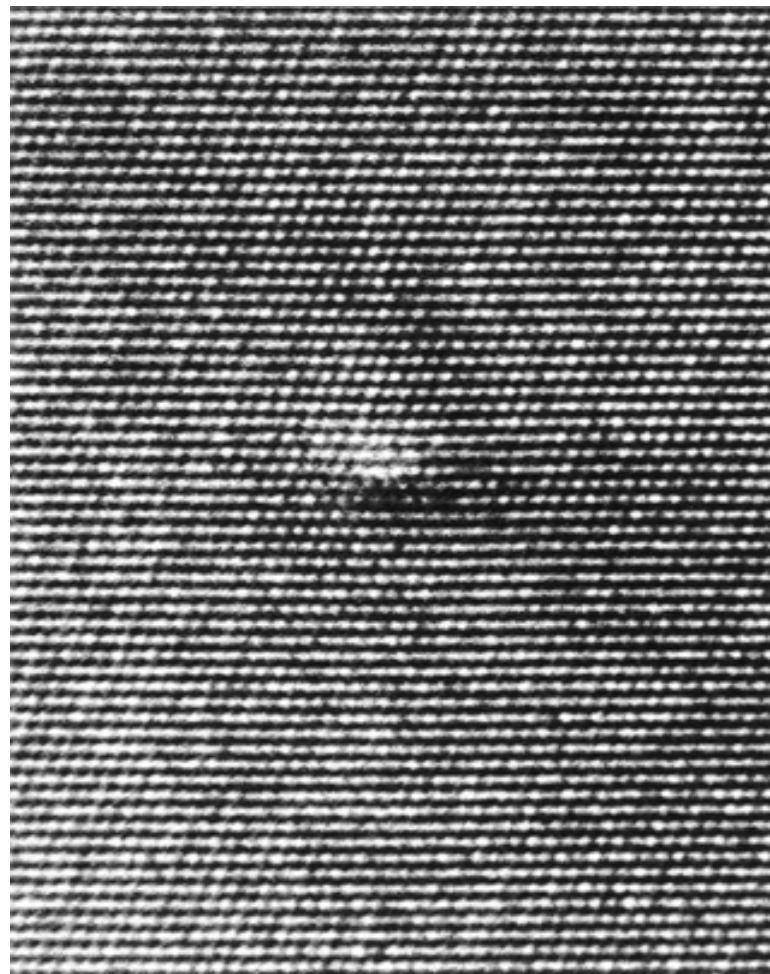
Steve Roberts – Microplasticity

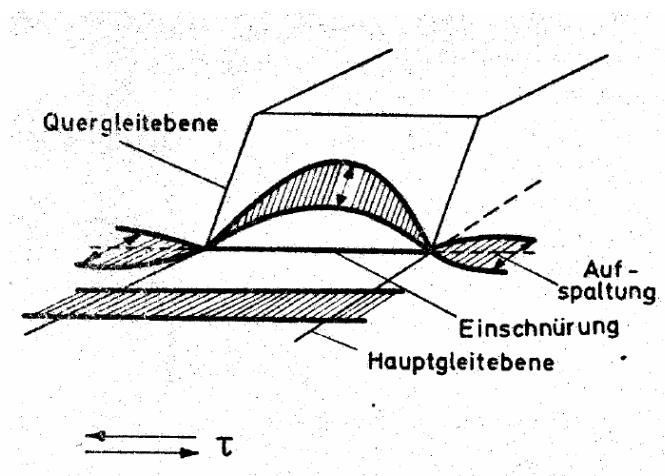
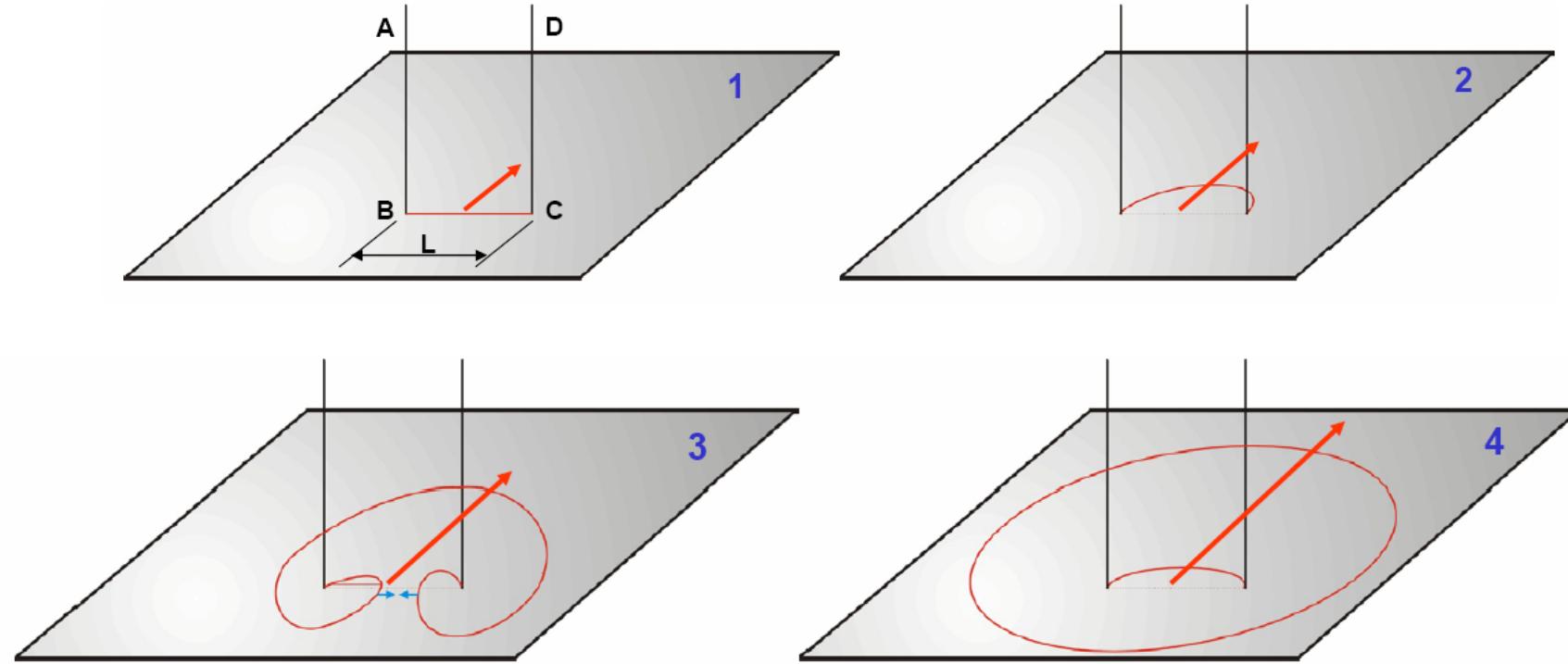
© S.G. Roberts





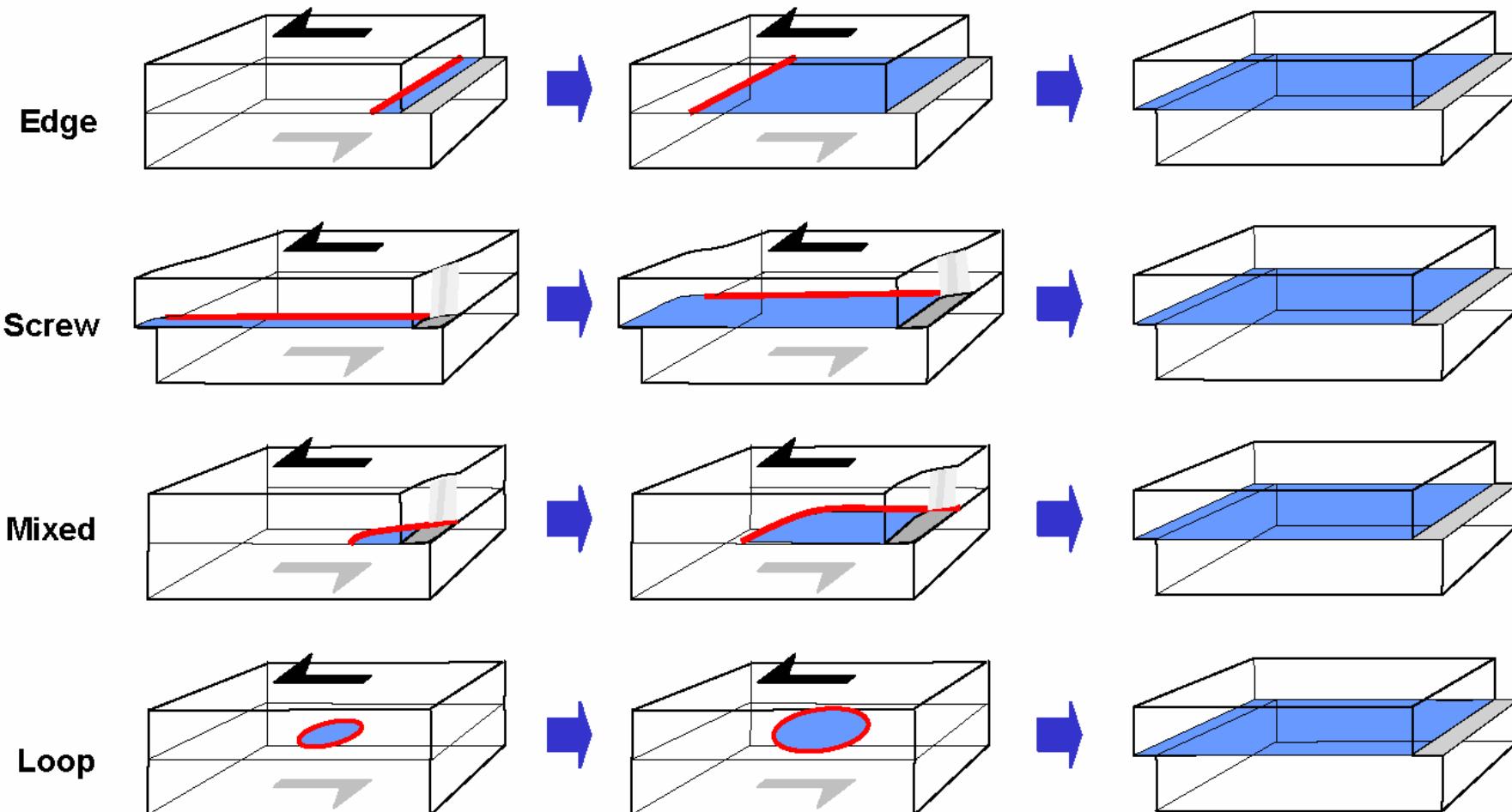






## dislocations

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## dislocations

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Displacement vector:

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

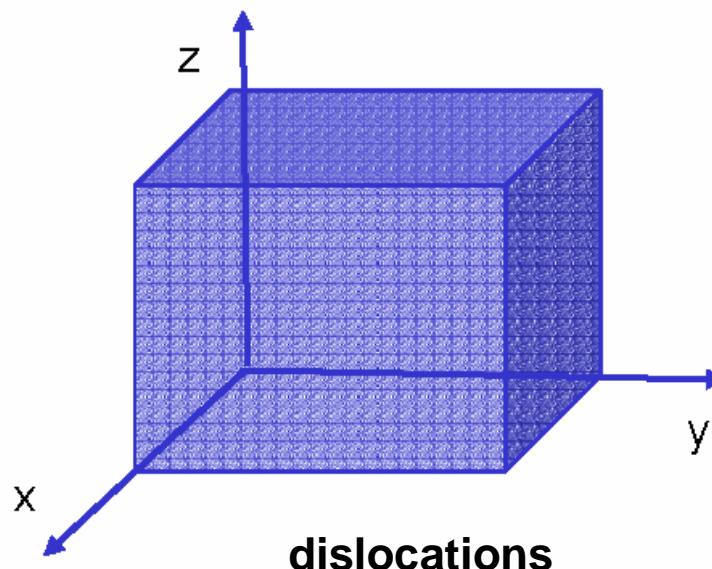
Strain tensor:

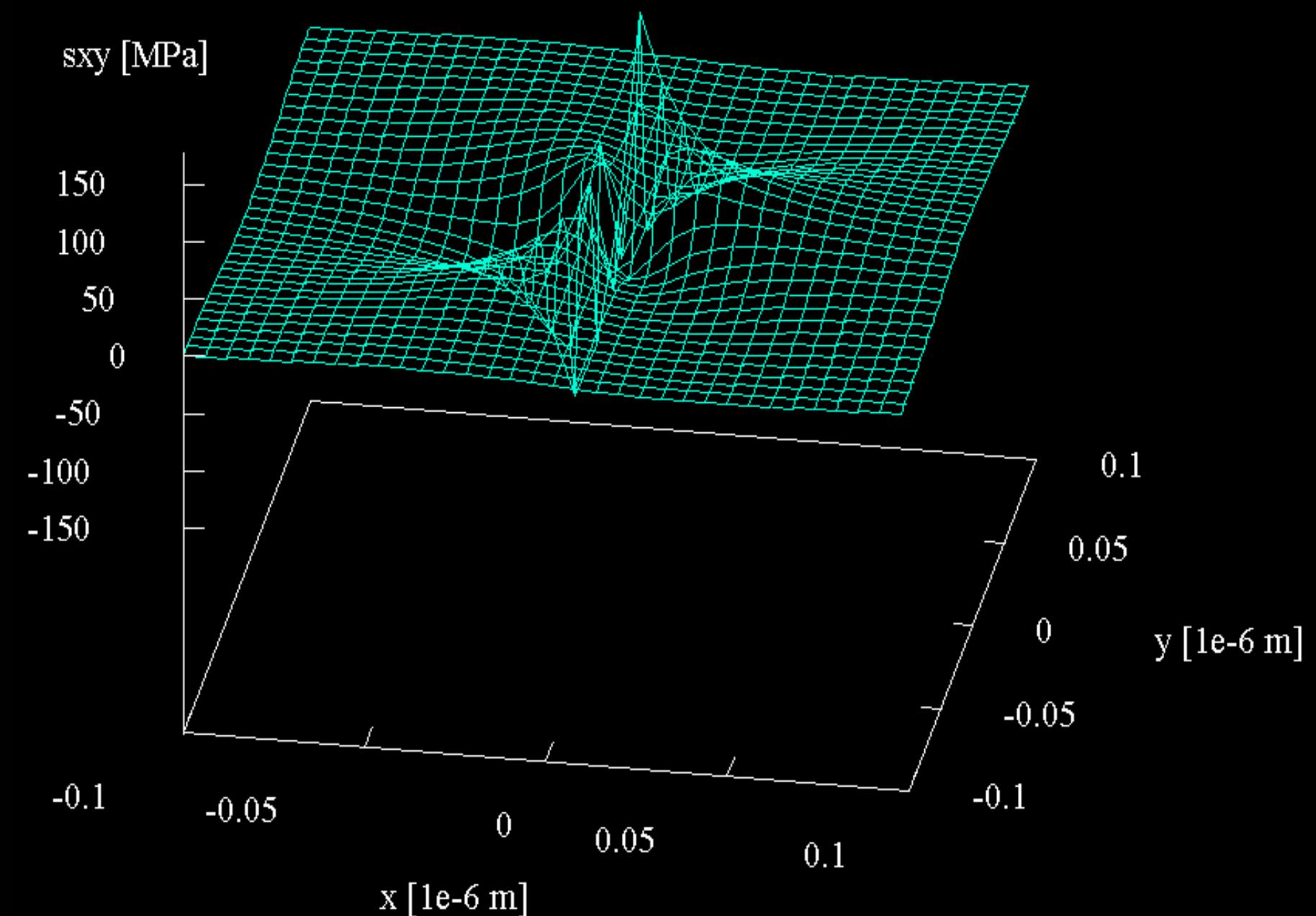
$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}$$

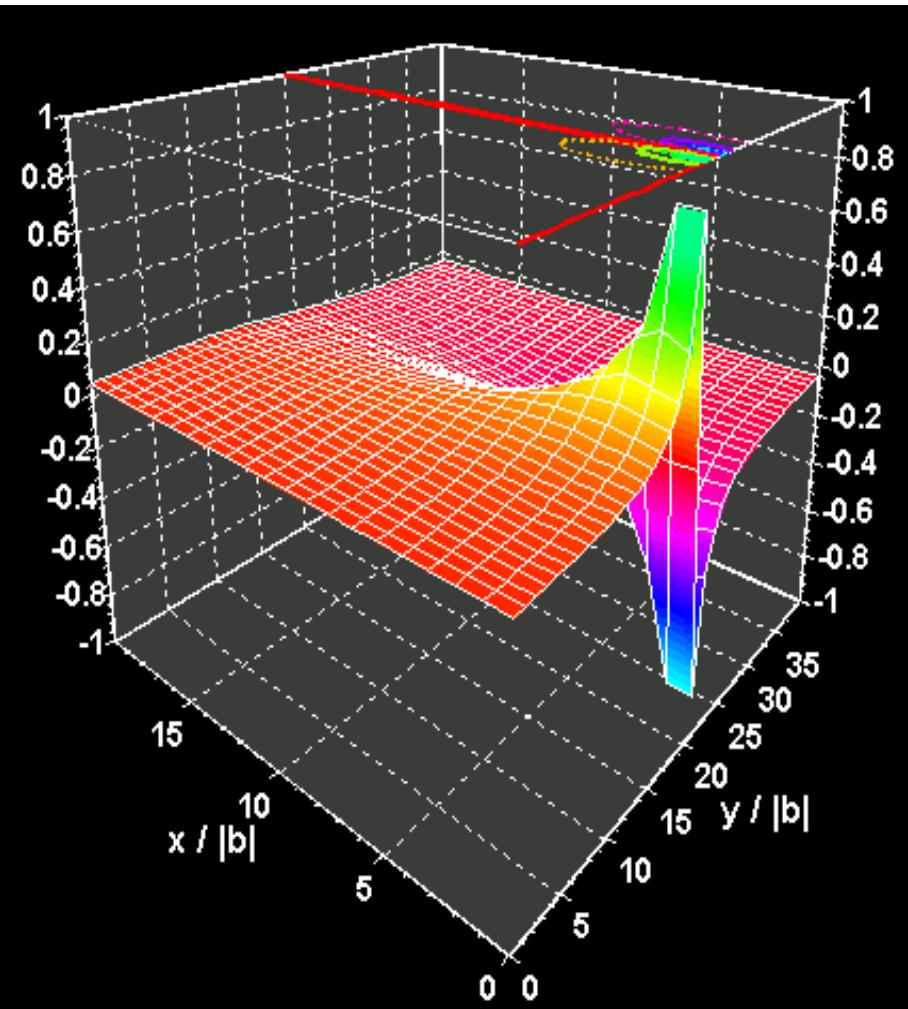
$$\varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right)_{etc.}$$

Dilatation,  $\Delta$ :

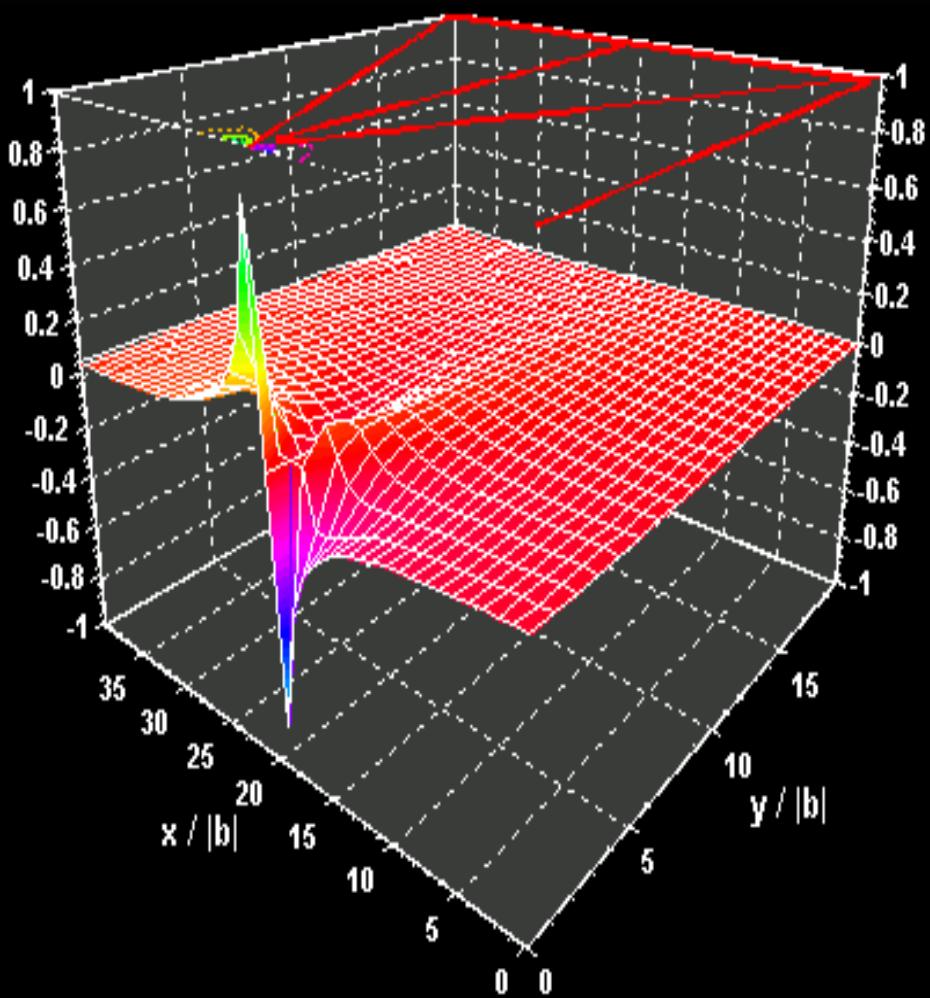
$$\Delta = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$







$$\sigma_{xx} / (Gb)/(2\pi)$$



$$\sigma_{xy} / (Gb)/(2\pi)$$