

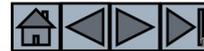
MSE2711  
**Materials Science**

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Hakan Yilmazer

Lecture 6 – Imperfections in the Atomic and  
Ionic Arrangements

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## Objectives of Chapter 4



- Introduce the three basic types of imperfections: point defects, line defects (or dislocations), and surface defects.
- Explore the nature and effects of different types of defects.

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## Chapter Outline



- 4.0 Defects
- 4.1 Point Defects
- 4.3 Linear Defects
- 4.4 Observing Defects
- 4.5 Significance of Linear Defects
- 4.6 Schmid' s Law
- 4.7 Influence of Crystal Structure
- 4.8 Surface Defects
- 4.9 Importance of Defects

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**Defects have a profound impact on the macroscopic properties of materials**



**Bonding**

+

**Structure**

+

**Defects**

→

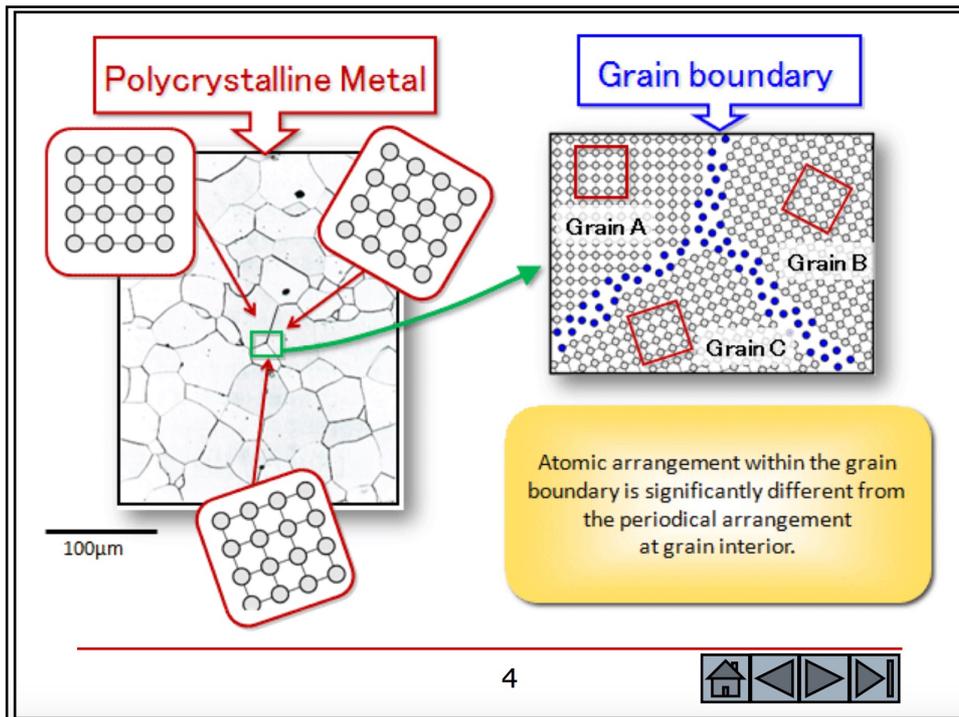
**Properties**

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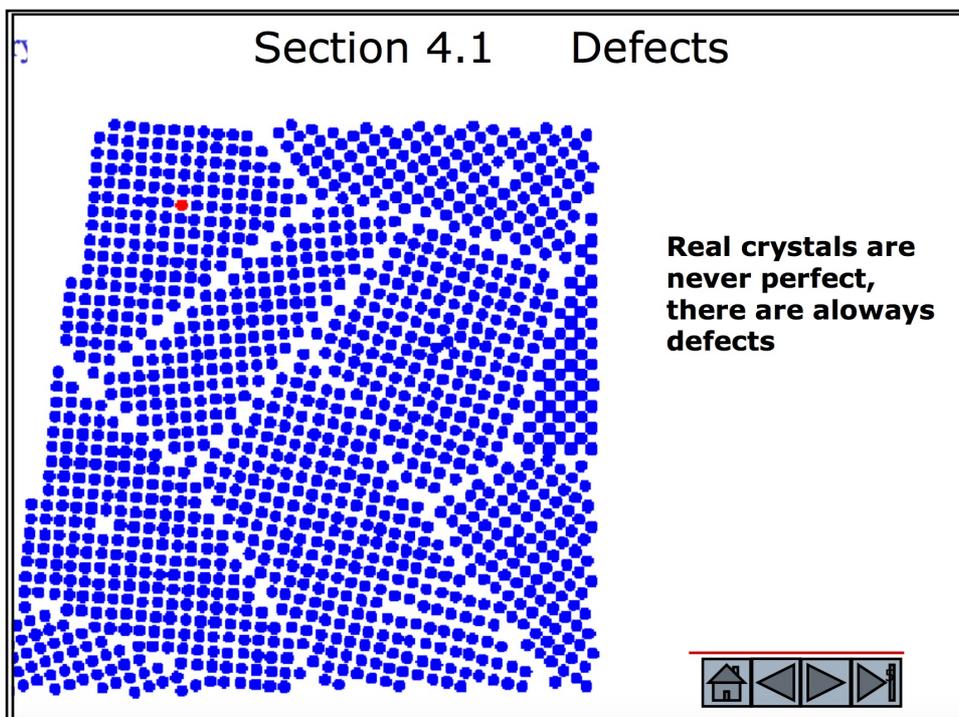
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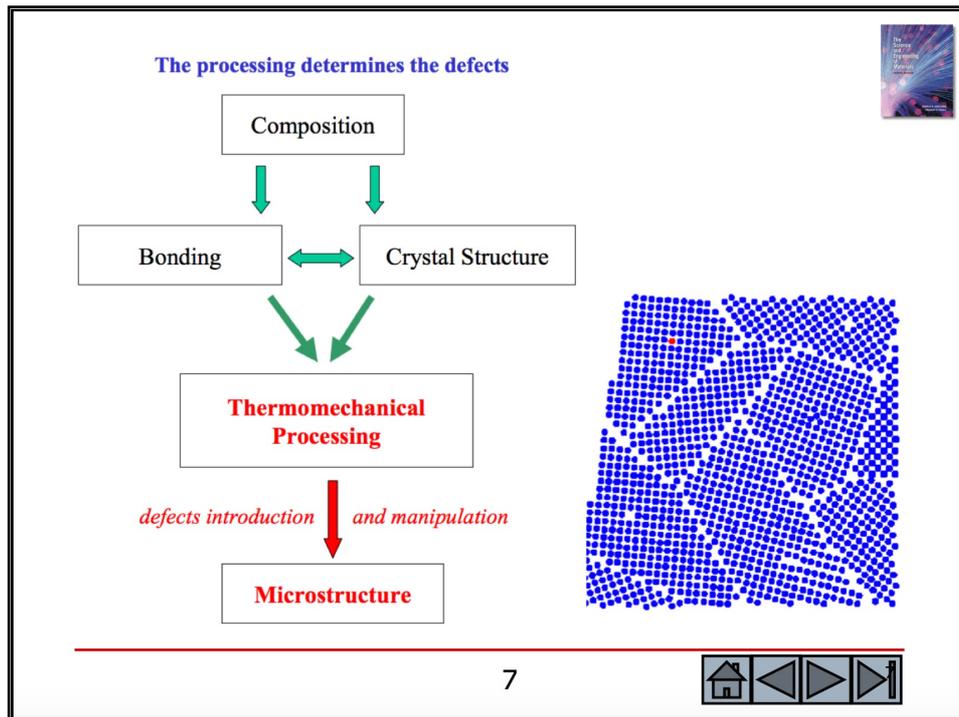
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## Types of Defects

Defects may be classified into four categories depending on their dimension:

- 0D, Point defects:** atoms missing or in irregular places in the lattice (vacancies, interstitials, impurities)
- 1D, Linear defects:** groups of atoms in irregular positions (e.g. screw and edge dislocations)
- 2D, Planar defects:** the interfaces between homogeneous regions of the material (grain boundaries, external surfaces)
- 3D, Volume defects:** extended defects (pores, cracks)

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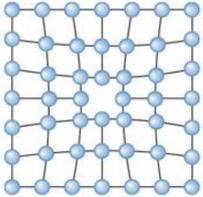
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## Section 4.1 Point Defects

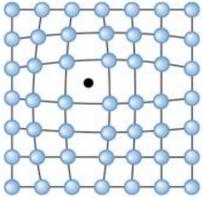


- **Point defects** - Imperfections, such as vacancies, that are located typically at one (in some cases a few) sites in the crystal.
- **Extended defects** - Defects that involve several atoms/ions and thus occur over a finite volume of the crystalline material (e.g., dislocations, stacking faults, etc.).
- **Vacancy** - An atom or an ion missing from its regular crystallographic site.
- **Interstitial defect** - A point defect produced when an atom is placed into the crystal at a site that is normally not a lattice point.
- **Substitutional defect** - A point defect produced when an atom is removed from a regular lattice point and replaced with a different atom, usually of a different size.

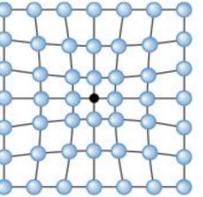




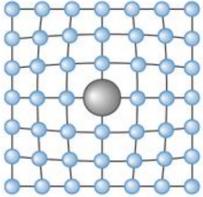
**vacancy (a)**



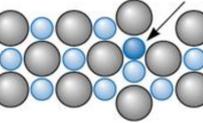
**(b)**  
**interstitial atom**



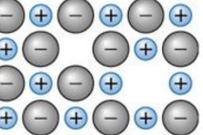
**(c)**  
**small substitutional atom**



**(d)**  
**large substitutional**



**(e)**  
**Frenkel defect**

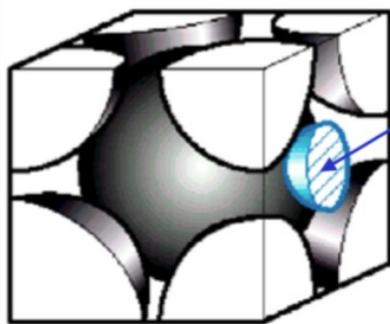


**(f)**  
**Schottky defect**

**Point defects change the crystal lattices, called " **distortion**".**



## Carburization in industry



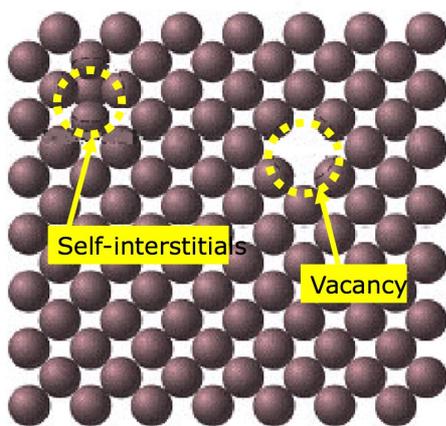
Carbon interstitial atom in BCC iron

□ Surface hardening

Interstitial solid solution of C in  $\alpha$ -Fe. The C atom is small enough to fit, after introducing some strain into the BCC lattice.

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## Point defects: vacancies & interstitials



**Vacancy** - lattice position that is vacant because atom is missing.

**Interstitial** - atom that occupies a place outside the normal lattice position. May be same type of atom (**self interstitial**) or an **impurity interstitial**.

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## How many vacancies?

**Equilibrium number of vacancies is due to thermal vibrations**

$$N_v = N_s \exp\left(-\frac{Q_v}{k_B T}\right)$$

**$N_s$**  = number of regular lattice sites  
 **$k_B$**  = Boltzmann constant  
 **$Q_v$**  = energy to form a vacant lattice site in a perfect crystal  
 **$T$**  = temperature in Kelvin (note, not in °C or °F).

Room temperature in copper: one vacancy per  $10^{15}$  atoms.  
 Just below the melting point: one vacancy for every 10,000 atoms.

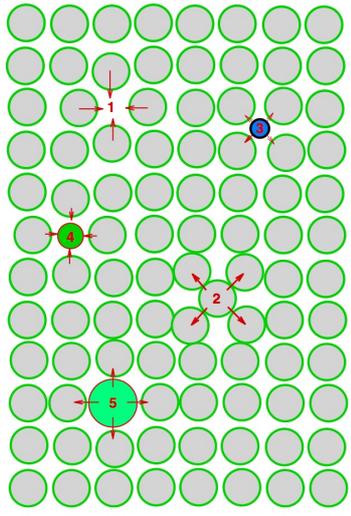
Above **lower bound** to number of vacancies. Additional (**non-equilibrium**) vacancies introduced in growth process or treatment (plastic deformation, quenching, etc.)

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## Point defects: self-interstitials, impurities



- (1) **vacancies**
- (2) **self-interstitial**
- (3) **interstitial impurity**
- (4,5) **substitutional impurities**

Arrows → local stress introduced by defect

### Self-interstitials

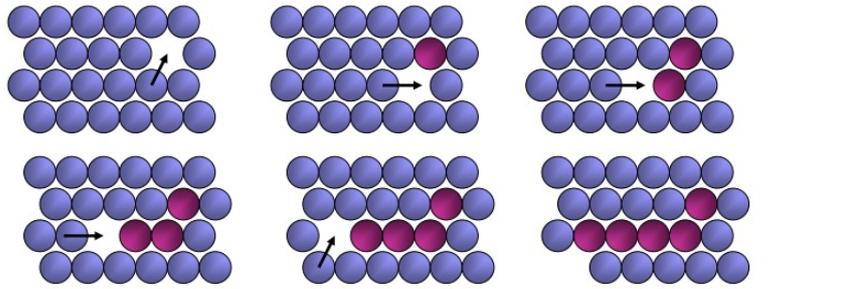
**Large distortions** in surrounding lattice  
 ⇒ **Energy** of self-interstitial formation is ~ 3 x larger than for vacancies ( $Q_i \sim 3 \times Q_v$ )  
 ⇒ equilibrium concentration of self-interstitials is very low (<  $1/ \text{cm}^3$  at 300K)

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## Vacancys



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### Örnek 4.2. Demirdeki Boşluk Konsantrasyonu



HMK yapıdaki demir kristalinin yoğunluğunun  $7.87 \text{ g/cm}^3$  olması için gerekli boşluk konsantrasyonunu hesaplayınız? Demir için latis parametresi  $2.866 \times 10^{-8} \text{ cm}$ .

#### ÇÖZÜM

Teorik yoğunluk latis parametresi ve atom ağırlığından hesaplanabilir.

Demirin atom ağırlığı:  
55.847 g/mol

$$\rho = \frac{(2 \text{ atoms/cell})(55.847 \text{ g/mol})}{(2.866 \times 10^{-8} \text{ cm})^3 (6.02 \times 10^{23} \text{ atoms/mol})} = 7.8814 \text{ g/cm}^3$$

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**ÇÖZÜM (Devamı)**

İstenilen yoğunluğa göre hücredeki atom sayısını belirleyelim:  $7.87 \text{ g/cm}^3$ :

$$\rho = \frac{(X \text{ atoms/cell})(55.847 \text{ g/mol})}{(2.866 \times 10^{-8} \text{ cm})^3(6.02 \times 10^{23} \text{ atoms/mol})} = 7.87 \text{ g/cm}^3$$

$$X \text{ atoms/cell} = \frac{(7.87)(2.866 \times 10^{-8})^3(6.02 \times 10^{23})}{55.847} = 1.9971$$

Bilindiği gibi hücredeki atom sayısı 2 olması beklenir. Dolayısıyla hücre başına  $2.00 - 1.9971 = 0.0029$  boşluk mevcuttur.  $1 \text{ cm}^3$  teki toplam boşluk:

$$\text{Vacancies/cm}^3 = \frac{0.0029 \text{ vacancies/cell}}{(2.866 \times 10^{-8} \text{ cm})^3} = 1.23 \times 10^{20}$$

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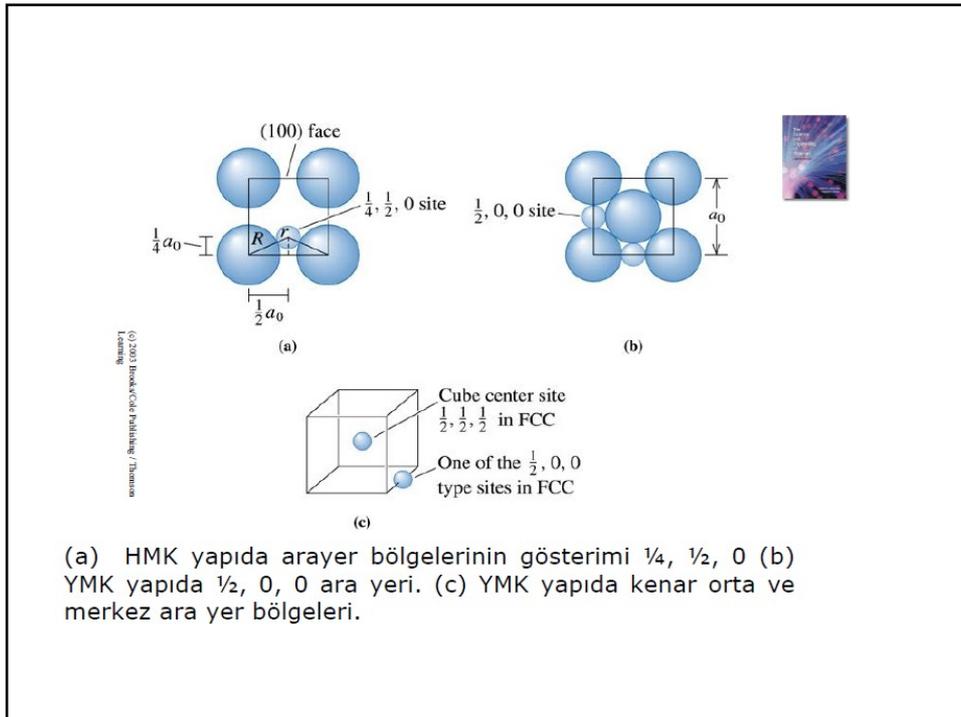
**Örnek 4.3. Demirdeki Karbon Bölgeleri**

YMK demirde, karbon atomları oktahedral bölgelerde ve hücrenin merkezinde yerleşmişlerdir. HMK demirde tetrahedral bölgelerde yerleşirler.

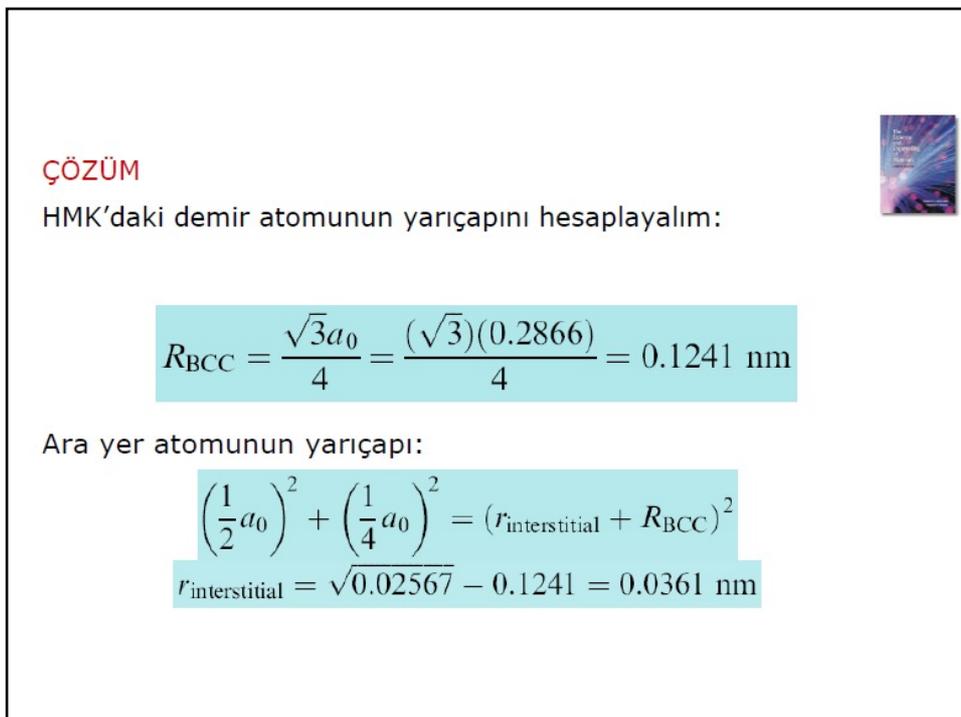
YMK latis parametresi  $0.3571 \text{ nm}$  HMK latis parametresi  $0.2866 \text{ nm}$ . Karbon atomlarının yarıçapı  $0.071 \text{ nm}$ .

(1) YMK yapıda mı yoksa HMK yapıda mı en yüksek distorsiyon görülür. (2) Tüm arayerler dolduğunda her iki kristal yapı için karbonların atomik yüzdesi ne olur?

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**ÇÖZÜM**

Aynı hesaplamalar YMK yapıdaki demir ve ara yer atomu için yapıldığında:

$$R_{\text{FCC}} = \frac{\sqrt{2}a_0}{4} = \frac{(\sqrt{2})(0.3571)}{4} = 0.1263 \text{ nm}$$

$$2r_{\text{interstitial}} + 2R_{\text{FCC}} = a_0$$

$$r_{\text{interstitial}} = \frac{0.3571 - (2)(0.1263)}{2} = 0.0522 \text{ nm}$$

Arayer bölgesi HMK da YMK dan daha küçüktür. Her iki bölgede karbondan küçük olduğundan C, HMK'yı YMK'dan daha fazla distorsiyona uğratar. Sonuçta, HMK arayerine YMK dan daha az atom girmesi beklenir.

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**ÇÖZÜM**

2. 24 arayer atomu için yer vardır ancak her bir bölge/yer birim hücrenin yüzeyinde bulunduğu için bu bölgelerin sadece yarısı bir hücreye aittir. Böylece: (24 bölge)(1/2) = 12 birim hücre başına ara yer bölgelerinin sayısı

HMK daki C'ların atomik yüzdesi:

$$\text{at \% C} = \frac{12 \text{ C atoms}}{12 \text{ C atoms} + 2 \text{ Fe atoms}} \times 100 = 86\%$$

YMK da ise oktahedral arayerlerin sayısı

(12 kenar) (1/4) + 1 merkez = 4 birim hücre başına arayer sayısı

YMK demirde C'nun atomik yüzdesi:

$$\text{at \% C} = \frac{4 \text{ C atoms}}{4 \text{ C atoms} + 4 \text{ Fe atoms}} \times 100 = 50\%$$

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### 4.3 Linear defects

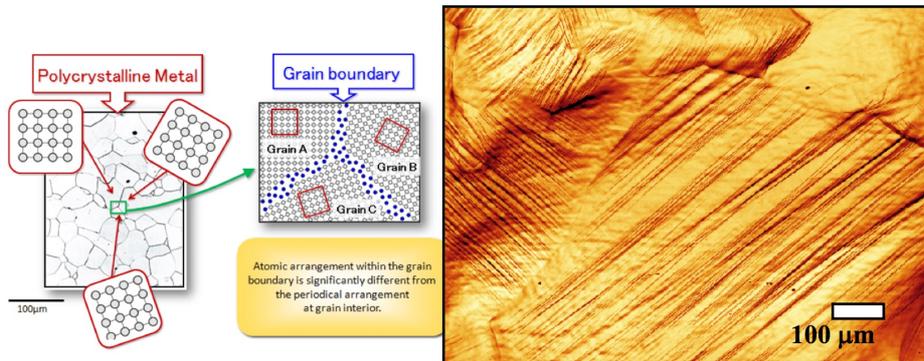


- ❑ **Dislocation** - A line imperfection in a crystalline material.
- ❑ **Screw dislocation** - A dislocation produced by skewing a crystal so that one atomic plane produces a spiral ramp about the dislocation.
- ❑ **Edge dislocation** - A dislocation introduced into the crystal by adding an ‘‘extra half plane’’ of atoms.
- ❑ **Mixed dislocation** - A dislocation that contains partly edge components and partly screw components.

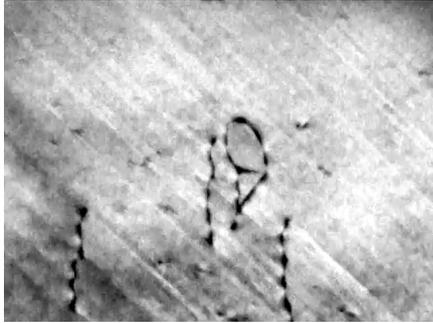


### Surface roughening of an AlMg(0.8%) alloy due to plastic deformation in tension

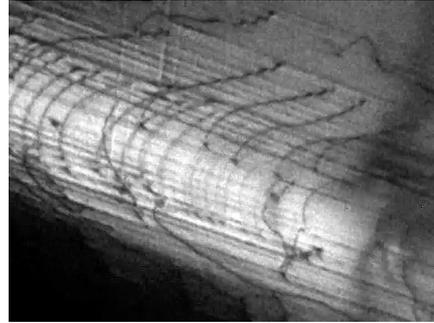
Image by confocal optical microscopy.  
Eric Moore, Ph.D. Thesis, UMBC 2006



## Dislocation motion



Dislocation generation through cross slip mechanism during in situ TEM deformation of alpha-titanium



Dislocation glide during in situ TEM straining at 400 C of 304 stainless steel

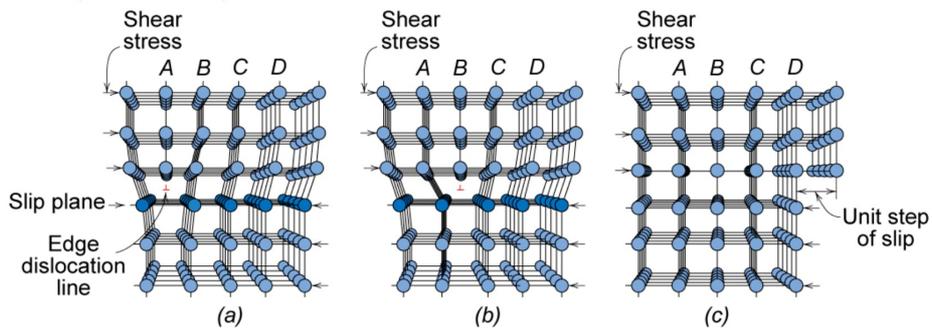
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## Dislocation Motion

### Dislocations & plastic deformation (PD)

- Cubic & hexagonal metals - plastic deformation by **plastic shear or slip** where one plane of atoms slides over adjacent plane by defect motion (dislocations).



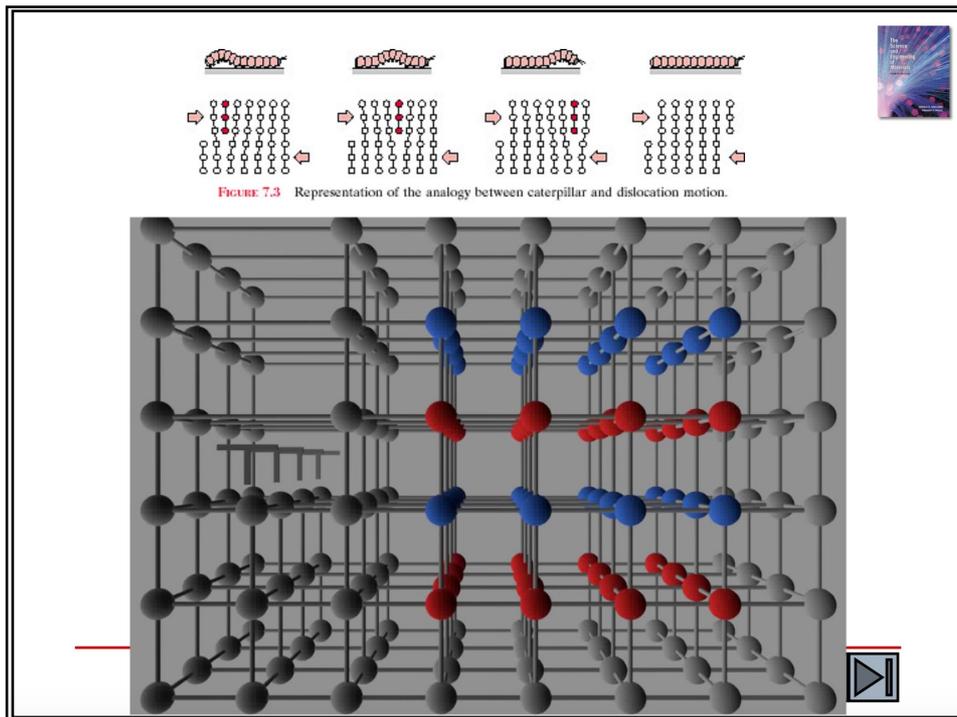
- If dislocations don't move, deformation doesn't occur!

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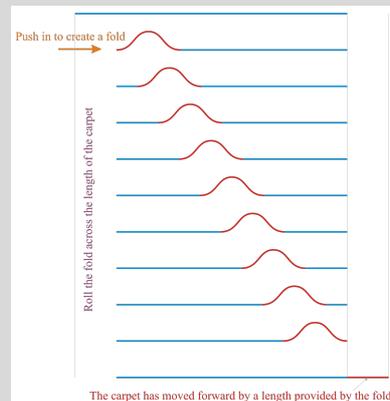
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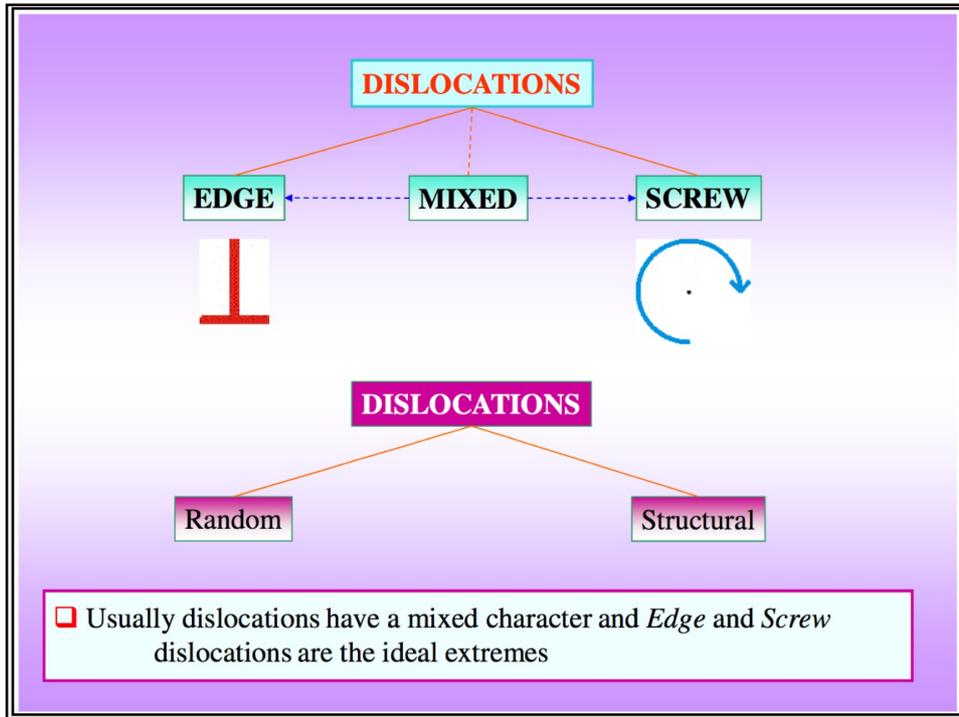
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- ❑ The analogy usually given to understand the role of dislocations in weakening a crystal is the one of 'pulling a carpet'.
- ❑ If one tries to pull an entire carpet (a long and wide one), by sliding it against the floor, the effort required is large.
- ❑ However, if a 'bump' is made in the carpet (as in the figure in the following slide) and this bump is moved across the length of the carpet, then the carpet moves forward by a small distance (as provided by the bump).
- ❑ The force required to move the bump will be considerably small as compared to the force required to pull the entire carpet.
- ❑ By creating and moving a series of bumps successively the carpet can be moved forward 'bit by bit'. (*Graphic on next slide*).



The 'carpet-pulling' analogy

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### Edge dislocation

(a)                      (b)                      (c)

Edge dislocation

**(a) The perfect crystal,**  
**(b) The perfect crystal is cut an extra plane of atoms is inserted**  
**(c) The bottom edge of the extra plane is an edge dislocation**

**A Burgers vector  $b$  is required to close a loop of equal atom spacings around the edge dislocation.**

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## Edge and dislocations

*Deformations of a hollow cylinder showing the formation of various defects (Volterra constructions)*

*Note that not only can dislocations be created this way; but also disclinations*

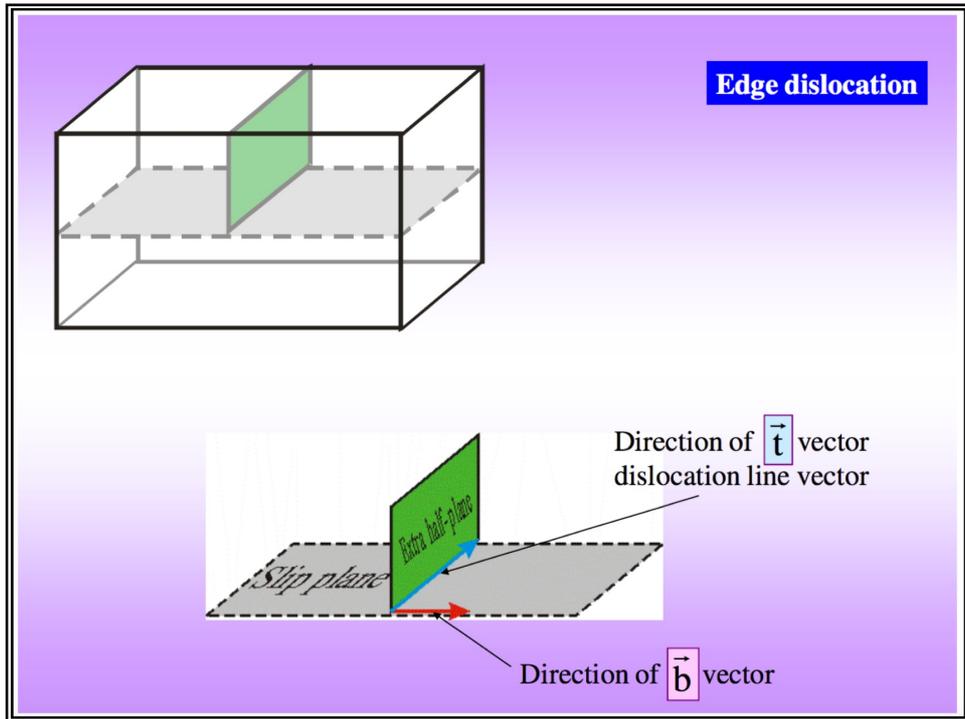
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**Burgers Vector**

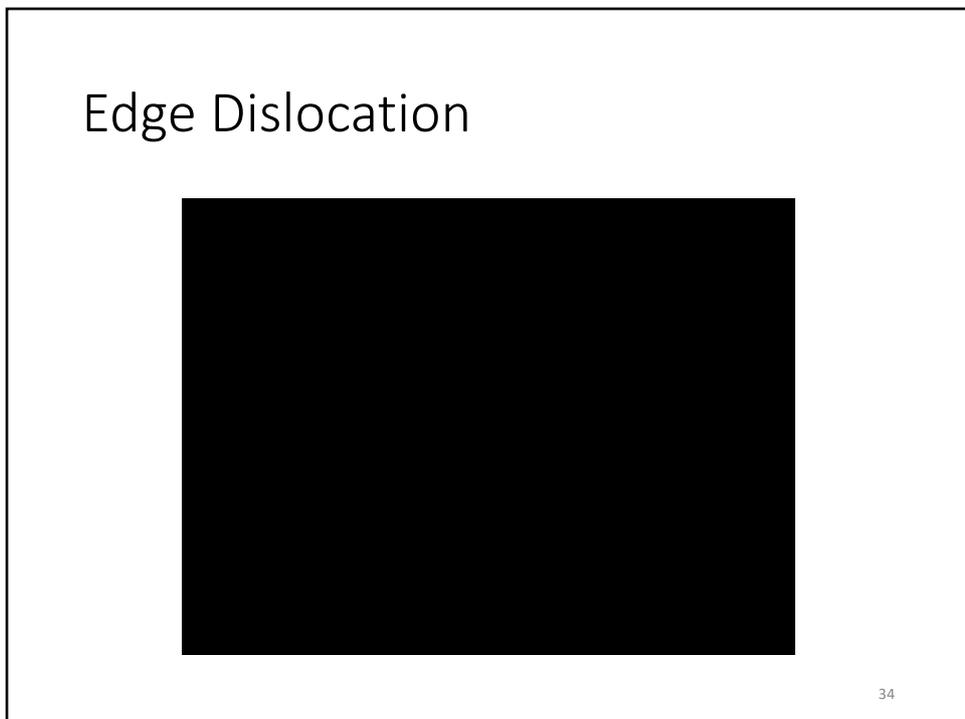
**Edge dislocation**

**RHFS:**  
Right Hand Finish to Start convention

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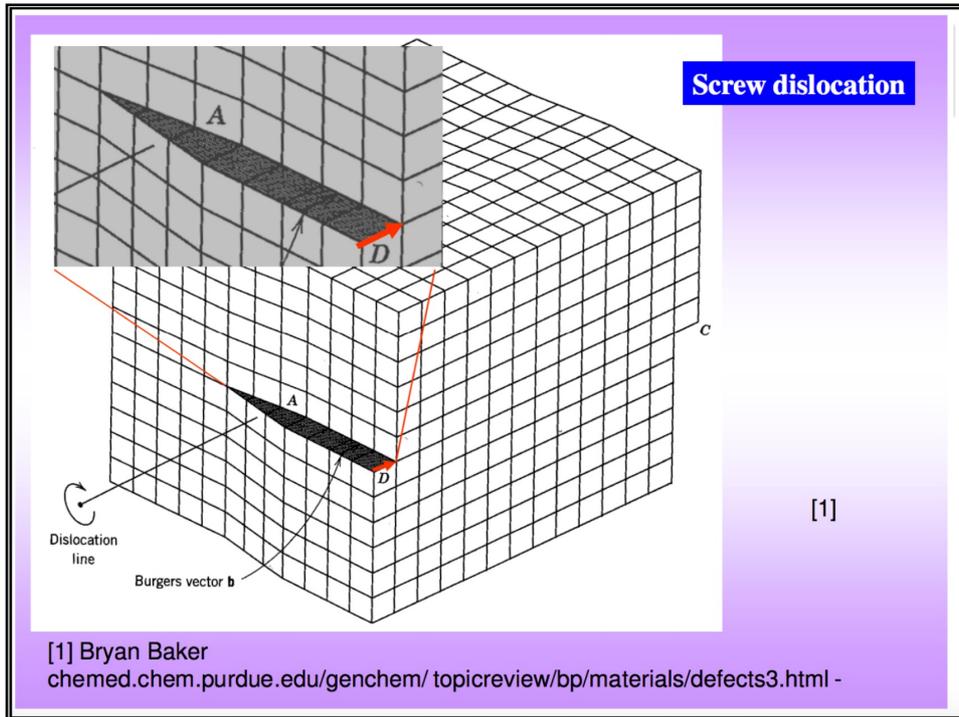
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- ❑ Dislocation is a boundary between the slipped and the unslipped parts of the crystal lying over a slip plane
- ❑ The intersection of the extra half-plane of atoms with the slip plane defines the dislocation line (*for an edge dislocation*)
- ❑ Direction and magnitude of slip is characterized by the Burgers vector of the dislocation (*A dislocation is born with a Burgers vector*)
- ❑ The Burgers vector is determined by the Burgers Circuit
- ❑ Right hand screw (finish to start) convention is used for determining the direction of the Burgers vector
- ❑ As the periodic force field of a crystal requires that atoms must move from one equilibrium position to another  $\Rightarrow \mathbf{b}$  must connect one lattice position to another (*for a full dislocation*)
- ❑ Dislocations tend to have as small a Burgers vector as possible

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- ❑ The edge dislocation has compressive stress field above and tensile stress field below the slip plane
- ❑ Dislocations are non-equilibrium defects and would leave the crystal if given an opportunity

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### Screw dislocation

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(a) (b) (c)

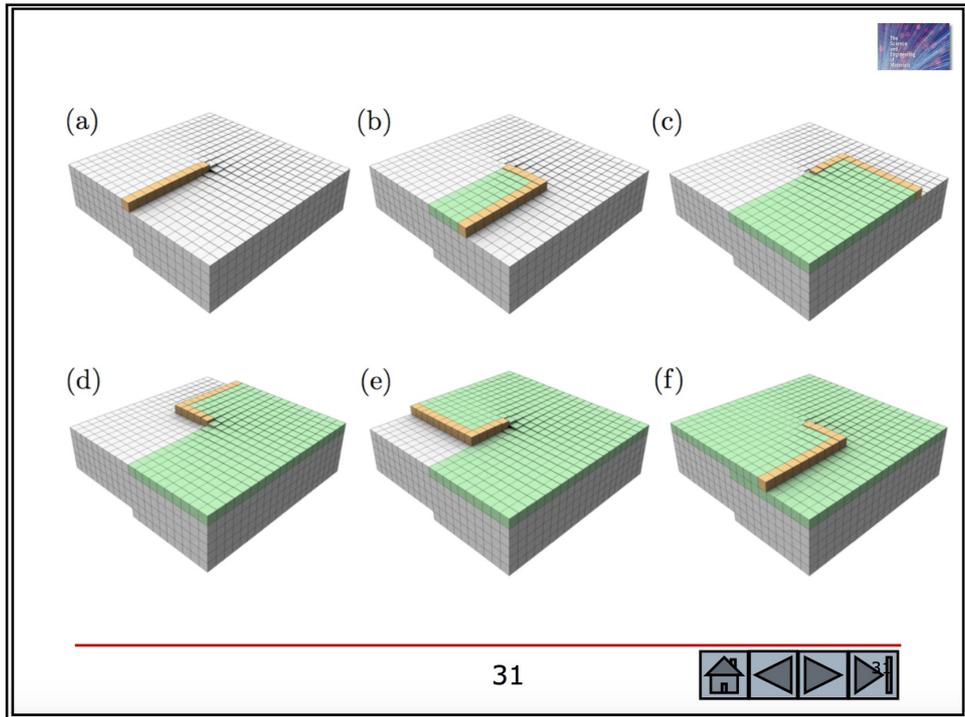
**(a) The perfect crystal,**  
**(b) The perfect crystal is cut**  
**(c) the cut crystal is sheared one atom spacing**

**The line along which shearing occurs is a screw dislocation.**

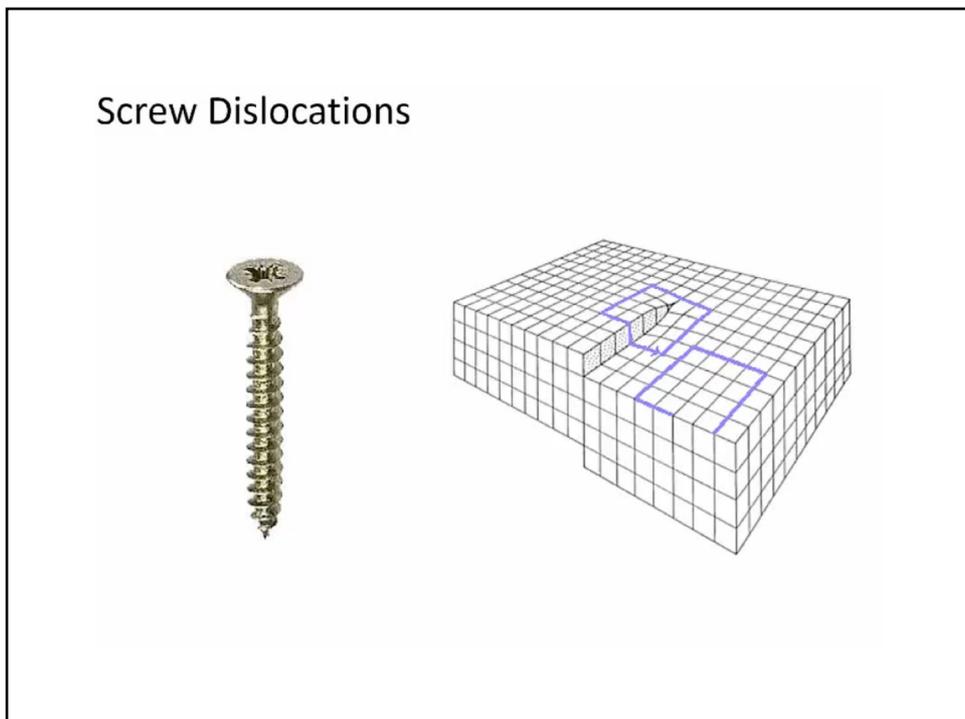
**A Burgers vector  $b$  is required to close a loop of equal atom spacings around the screw dislocation.**

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**Geometric properties of dislocations**

Dislocation Property	Type of dislocation	
	Edge	Screw
Relation between dislocation line ( <b>t</b> ) and <b>b</b>	⊥	∥
Slip direction	∥ to <b>b</b>	∥ to <b>b</b>
Direction of dislocation line movement relative to <b>b</b>	∥	⊥
Process by which dislocation may leave slip plane	climb	Cross-slip

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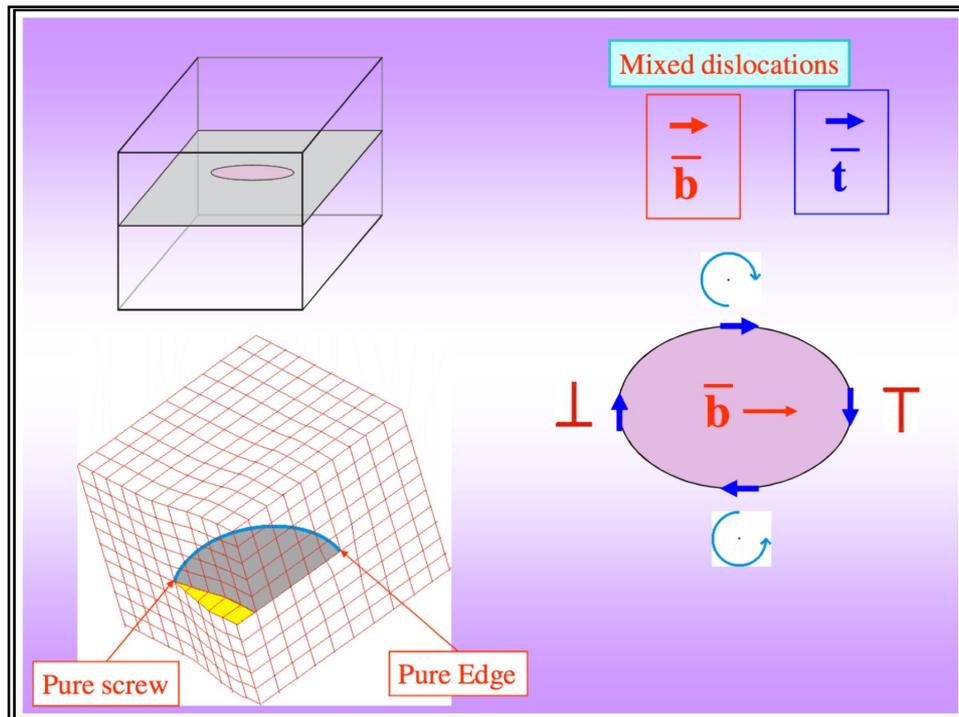
### A mixed dislocation

The screw dislocation at the front face of the crystal gradually changes to an edge dislocation at the side of the crystal.

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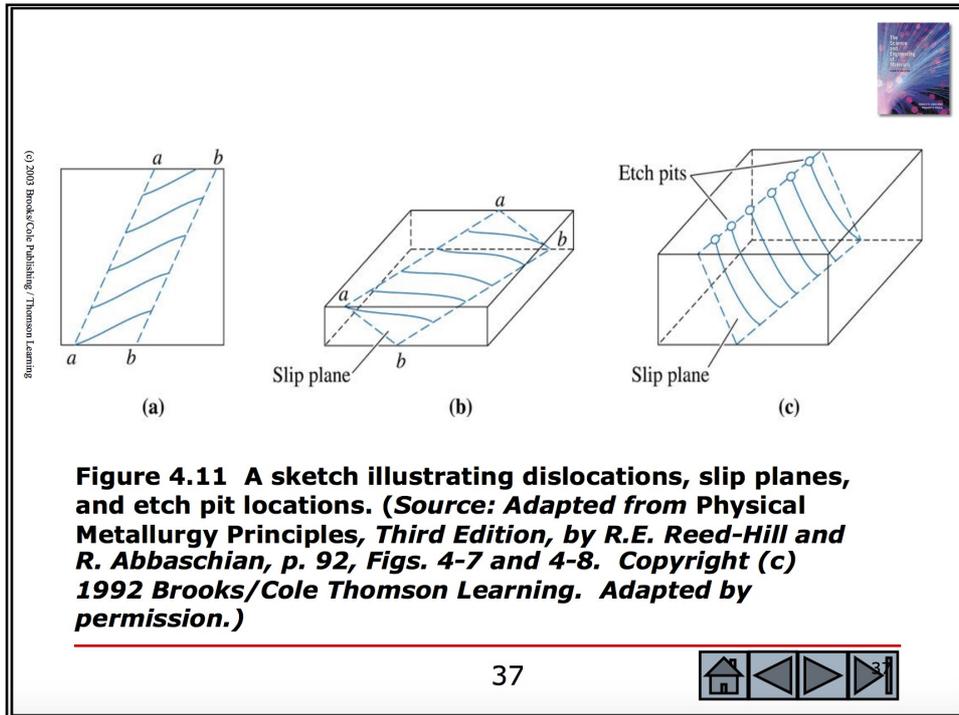
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## Section 4.4 Observing Dislocations

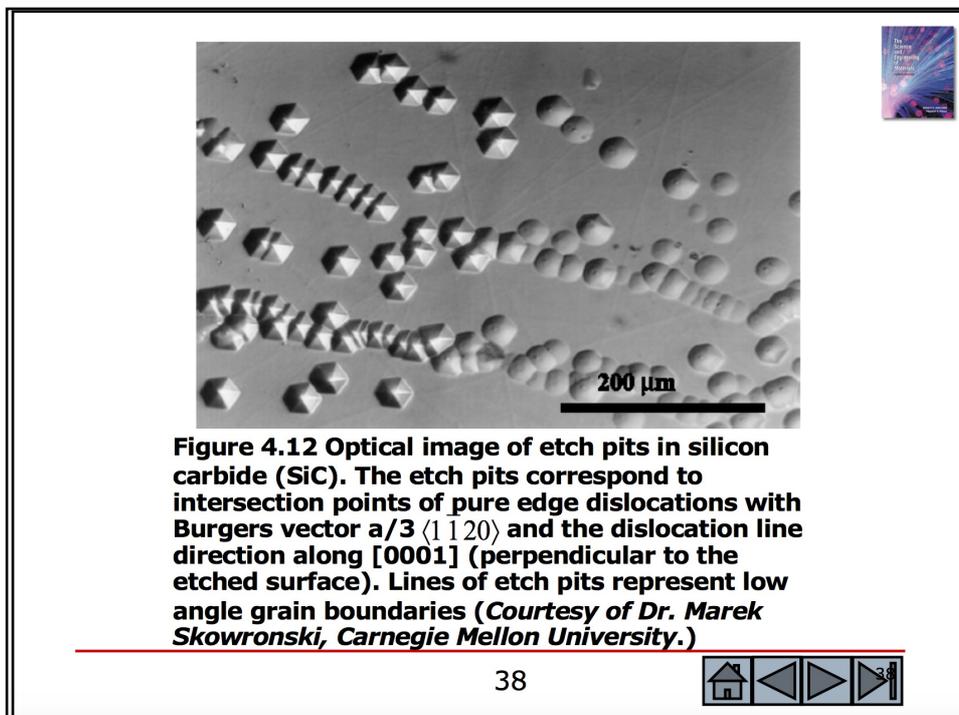
- **Etch pits** - Tiny holes created at areas where dislocations meet the surface. These are used to examine the presence and number density of dislocations.
- **Slip line** - A visible line produced at the surface of a metallic material by the presence of several thousand dislocations.
- **Slip band** - Collection of many slip lines, often easily visible.

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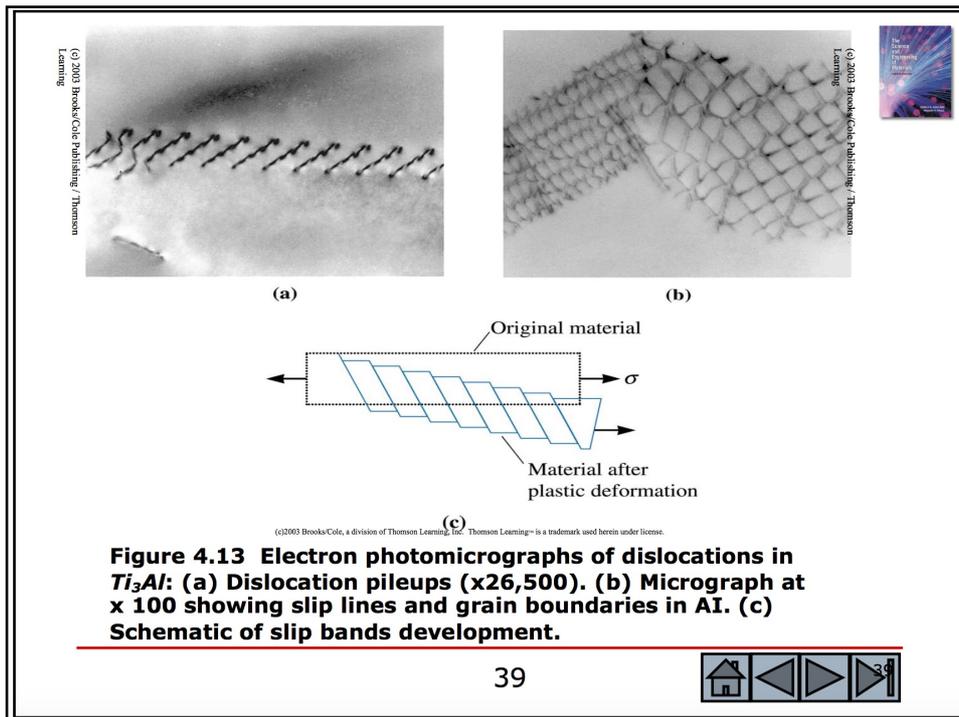
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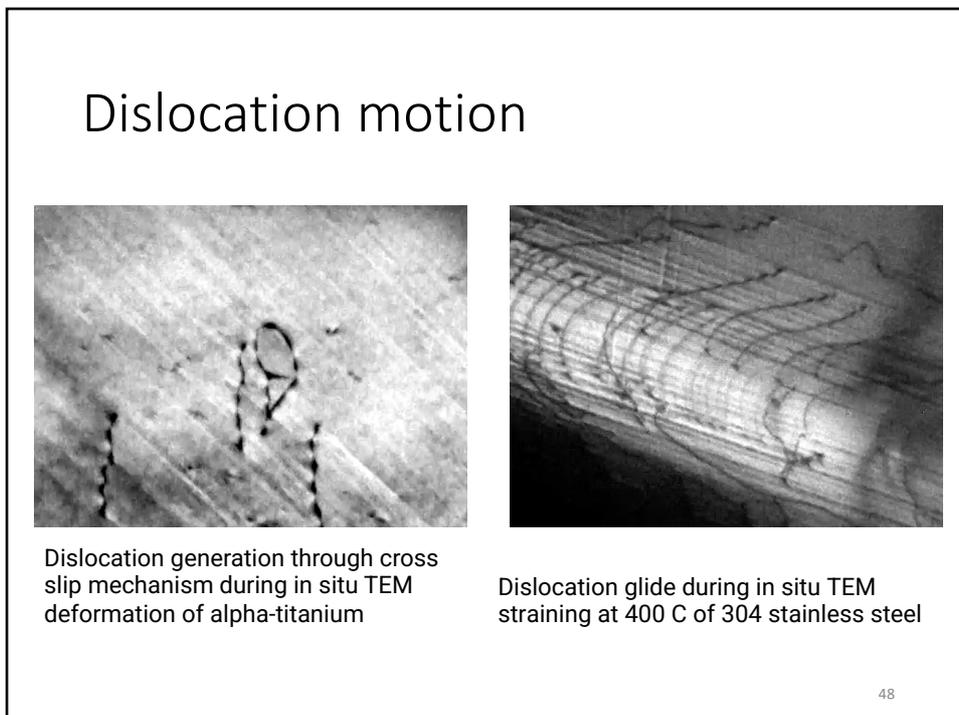
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## Dislocations & Materials Classes

**Dislocation types: edge and screw**

- **Metals: Dislocation motion easier.**
  - non-directional bonding
  - close-packed directions for slip.
- **Covalent Ceramics** (Si, diamond): **Motion hard.**
  - very hard,  $T_m > 3550\text{C}$
  - directional bonding
- **Ionic Ceramics (NaCl):** **Motion hard.**
  - need to avoid ++ and -- neighbors.
  - non-directional bonding

electron cloud

ion cores

**PD corresponds to the motion of large numbers of dislocations**

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Original defect-free crystal

Elastic deformation (ED): bonds are compressed and stretched, but not broken.

Plastic deformation (PD) by the introduction of dislocations.

Dislocations organize into parallel lines, forming low-angle grain boundaries.

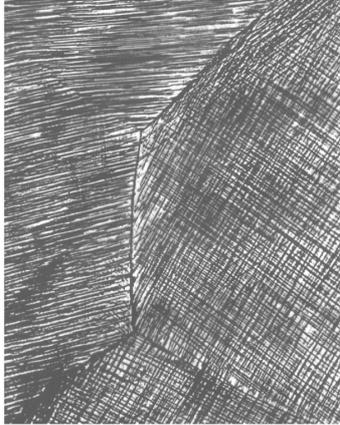
Recrystallization via annealing: defect free sample with new shape is obtained.

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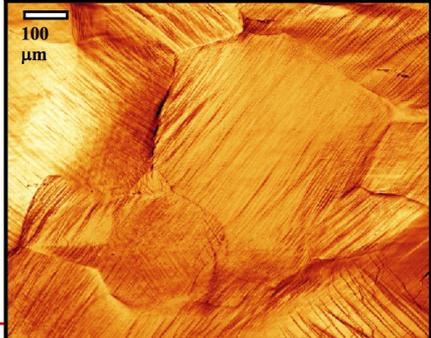
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## Deformation Mechanisms

### Slip



**Slip lines in Al**  
The orientation of the individual crystallite determines which slip system(s) are active.



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## Slip

**Slip System: Slip planes and directions**

- **Slip plane** - plane allowing easiest slippage
  - Highest planar densities
- **Slip direction** - direction of movement
  - - Highest linear densities

Slip is favored on closed packed planes since a lower shear stress for atomic displacement is required than for less densely packed planes.

Slip in the closed packed direction is also favored since less energy is required to move the atoms from one position to another if the atoms are closer together.

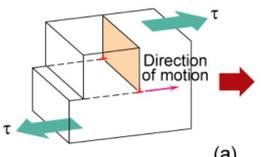
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## Dislocation Motion

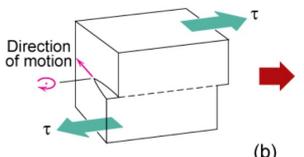
**Slip** is the process by which plastic deformation is produced by dislocation motion

- ❑ Dislocation moves along **slip plane** in **slip direction** perpendicular to dislocation line( **slip system**)
- ❑ Slip direction have the same direction as **Burgers vector**



(a)

**Edge dislocation**



(b)

**Screw dislocation**

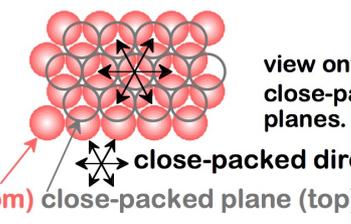
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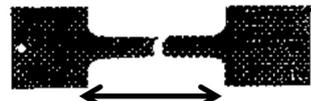
## Slip-Dislocation motion & CRYSTAL STRUCTURE

- Structure: **close-packed** planes & directions are preferred.

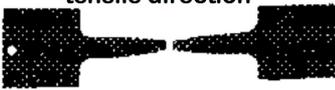


view onto two close-packed planes.  
close-packed plane (bottom) close-packed plane (top)  
close-packed directions

- Comparison among crystal structures:  
**FCC: many close-packed planes/directions;**  
**HCP: only one plane, 3 directions;**  
**BCC: none**



Mg (HCP)



Al (FCC)

tensile direction

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## Preferred slip systems for some metals

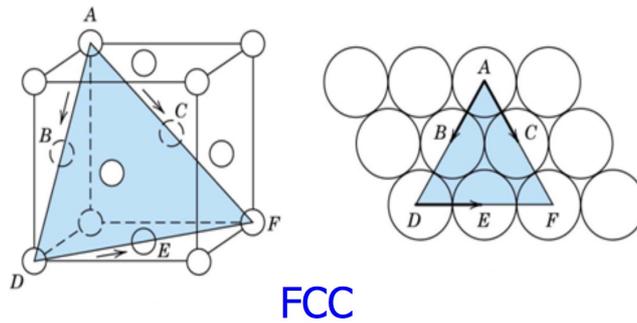
Metal	Crystal structure	Purity, %	Slip plane	Slip direction	Critical shear stress, MPa
Zn	hcp	99.999	(0001)	$[11\bar{2}0]$	0.18
Mg	hcp	99.996	(0001)	$[1120]$	0.77
Cd	hcp	99.996	(0001)	$[11\bar{2}0]$	0.58
Ti	hcp	99.99	(1010)	$[11\bar{2}0]$	13.7
Ag	fcc	99.9	(1010)	$[11\bar{2}0]$	90.1
		99.99	(111)	$[110]$	0.48
		99.97	(111)	$[110]$	0.73
		99.93	(111)	$[110]$	1.3
Cu	fcc	99.999	(111)	$[110]$	0.65
		99.98	(111)	$[110]$	0.94
Ni	fcc	99.8	(111)	$[110]$	5.7
Fe	bcc	99.96	(110)	$[111]$	27.5
			(112)		
			(123)		
Mo	bcc	...	(110)	$[111]$	49.0

48



55

## Slip System



- FCC Slip occurs on  $\{111\}$  planes (close-packed) in  $\langle 110 \rangle$  directions (close-packed)  
=> total of 12 slip systems in FCC
- in BCC & HCP other slip systems occur

49



56

(111)       $(\bar{1}11)$        $(1\bar{1}1)$        $(11\bar{1})$

Parallel

(111)

50

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So, for (111) plane:

(111),  $[10\bar{1}]$  or  $[\bar{1}01]$ ---1

(111),  $[1\bar{1}0]$  or  $[\bar{1}10]$ ---2

(111),  $[01\bar{1}]$  or  $[0\bar{1}1]$ ---3

**Therefore, for an FCC structure:  
 $\{111\} - \langle 110 \rangle$  , there are 12 slip systems.**

51

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### To sum up:

- ❑ Slip phenomenon is used to explain the plastic behaviour of materials.
- ❑ Slip occurs along certain crystal planes and directions.
- ❑ Slip planes & slip directions make slip systems.

Crystal system	Slip plane	Slip direction	Total number of slip systems	Active slip systems
fcc	{111}	<110>	12	5
hcp	{0001}	<2110>	3	2/3
bcc	{110} {100}	<111>	48	2

52



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## Section 4.6 Schmid's Law

- ❑ **Schmid's law** -The relationship between shear stress, the applied stress, and the orientation of the slip system—that is,

$$\tau = \sigma \cos \lambda \cos \phi$$

- ❑ **Critical resolved shear stress** - The shear stress required to cause a dislocation to move and cause slip.

53



60

### Surface roughening of an $\text{AlMg}(0.8\%)$ alloy due to plastic deformation in tension

Image by confocal optical microscopy.  
Eric Moore, Ph.D. Thesis, UMBC 2006

The diagram on the left shows a polycrystalline metal with a grain boundary. It includes a 100µm scale bar and a callout box stating: "Atomic arrangement within the grain boundary is significantly different from the periodical arrangement at grain interior." The microscopy image on the right shows a surface with diagonal striations and a 100µm scale bar.

54

61

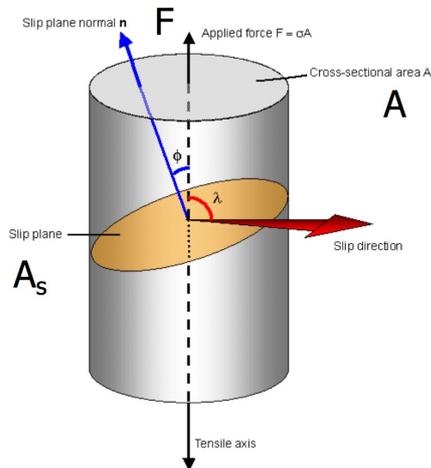
### Single Crystal Slip

The diagram on the left shows a blue cylinder with a pink arrow pointing up labeled "Direction of force" and a pink arrow pointing down. An orange helical band around the cylinder is labeled "Slip plane". The microscopy image on the right shows a vertical surface with a series of horizontal, slightly curved white lines on a dark background.

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62

❖ The stress that initiates slip is known as **the critical resolved shear stress.**



$\phi$ : Angle between the normal to the slip plane and the applied stress directions.

$\lambda$ : Angle between the slip and stress directions.

$$\tau_{CR} = \sigma \cdot \cos \lambda \cdot \cos \phi$$

56



63

### Stress and Dislocation Motion

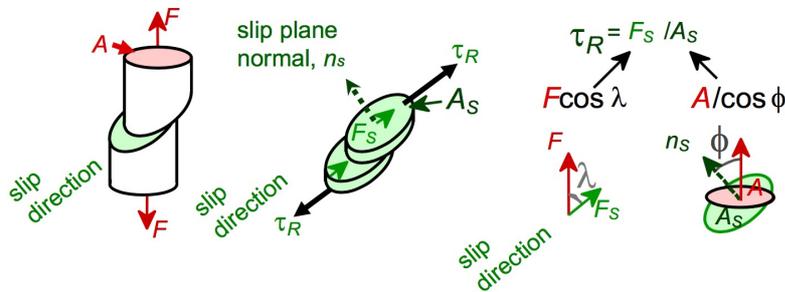


- Crystals slip due to a **resolved shear stress,  $\tau_R$** .
- Applied tension can produce such a stress.

**Applied tensile stress:**  $\sigma = F/A$

**Resolved shear stress:**  $\tau_R = F_s/A_s$

**Relation between  $\sigma$  and  $\tau_R$**



$$\tau_R = \sigma \cos \lambda \cos \phi$$

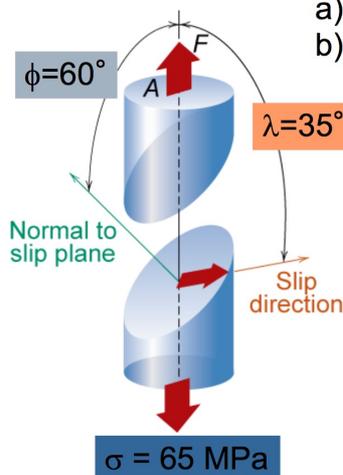
57



57

64

## Ex: Deformation of single crystal



- a) Will the single crystal yield?  
b) If not, what stress is needed?

$$\tau_{\text{crss}} = 30 \text{ MPa}$$

$$\tau = \sigma \cos \lambda \cos \phi$$

$$\sigma = 65 \text{ MPa}$$

$$\begin{aligned} \tau &= (65 \text{ MPa}) (\cos 35^\circ) (\cos 60^\circ) \\ &= (65 \text{ MPa}) (0.41) \end{aligned}$$

$$\tau = 26.62 \text{ MPa} < \tau_{\text{crss}} = 30 \text{ MPa}$$

So the applied stress of 65 MPa will not cause the crystal to yield.

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65

## Ex: Deformation of single crystal

What stress *is* necessary (i.e., what is the yield stress,  $\sigma_y$ )?

$$\tau_{\text{crss}} = 30 \text{ MPa} = \sigma_y \cos \lambda \cos \phi = \sigma_y (0.41)$$

$$\therefore \sigma_y = \frac{\tau_{\text{crss}}}{\cos \lambda \cos \phi} = \frac{30 \text{ MPa}}{0.41} = \underline{\underline{73.25 \text{ MPa}}}$$

So for deformation to occur the applied stress must be greater than or equal to the yield stress

$$\sigma \geq \sigma_y = 73.25 \text{ MPa}$$

60



66

## Ex: Deformation of single crystal



Consider a single crystal of BCC iron oriented such that a tensile stress is applied along a  $[010]$  direction.

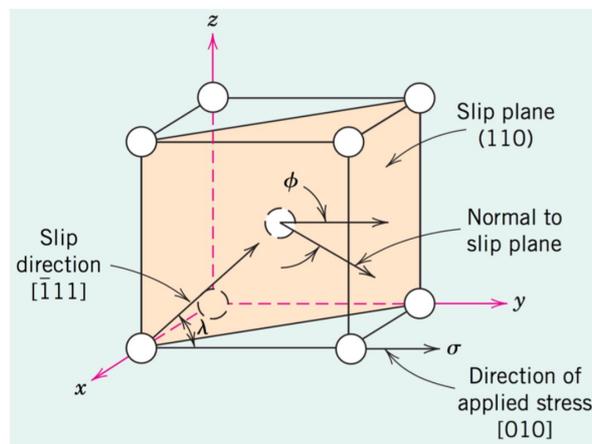
- (a) Compute the resolved shear stress along a  $(110)$  plane and in a  $[-111]$  direction when a tensile stress of 52 MPa is applied.
- (b) If slip occurs on a  $(110)$  plane and in a  $[-111]$  direction, and the critical resolved shear stress is 30 MPa, calculate the magnitude of the applied tensile stress necessary to initiate yielding.

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## Ex: Deformation of single crystal



62



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## Ex: Deformation of single crystal



- A BCC unit cell along with the slip direction and plane as well as the direction of the applied stress are shown in the accompanying diagram. In order to solve this problem, we must use Schmid Equation.
- However, it is first necessary to determine values for  $\phi$  and  $\lambda$ , where, from this diagram,  $\phi$  is the angle between the normal to the (110) slip plane (i.e., the [110] direction) and the [010] direction, and  $\lambda$  represents the angle between the [-111] and [010] directions. In general, for cubic unit cells, the angle  $\theta$  between directions 1 and 2, represented by  $[u_1v_1w_1]$  and  $[u_2v_2w_2]$ , respectively, is given by

$$\theta = \cos^{-1} \left[ \frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)(u_2^2 + v_2^2 + w_2^2)}} \right]$$

63



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## Ex: Deformation of single crystal



For the determination of the value of  $\phi$ , let  $[u_1v_1w_1] = [110]$  and  $[u_2v_2w_2] = [010]$ , such that

$$\begin{aligned} \phi &= \cos^{-1} \left\{ \frac{(1)(0) + (1)(1) + (0)(0)}{\sqrt{[(1)^2 + (1)^2 + (0)^2][(0)^2 + (1)^2 + (0)^2]}} \right\} \\ &= \cos^{-1} \left( \frac{1}{\sqrt{2}} \right) = 45^\circ \end{aligned}$$

However, for  $\lambda$ , we take  $[u_1v_1w_1] = [\bar{1}11]$  and  $[u_2v_2w_2] = [010]$ , and

$$\begin{aligned} \lambda &= \cos^{-1} \left[ \frac{(-1)(0) + (1)(1) + (1)(0)}{\sqrt{[(-1)^2 + (1)^2 + (1)^2][(0)^2 + (1)^2 + (0)^2]}} \right] \\ &= \cos^{-1} \left( \frac{1}{\sqrt{3}} \right) = 54.7^\circ \end{aligned}$$

Thus, according to Equation 7.2,

$$\begin{aligned} \tau_R &= \sigma \cos \phi \cos \lambda = (52 \text{ MPa})(\cos 45^\circ)(\cos 54.7^\circ) \\ &= (52 \text{ MPa}) \left( \frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{3}} \right) \\ &= 21.3 \text{ MPa (3060 psi)} \end{aligned}$$

(b) The yield strength  $\sigma_y$  may be computed from Equation 7.4;  $\phi$  and  $\lambda$  are the same as for part (a), and

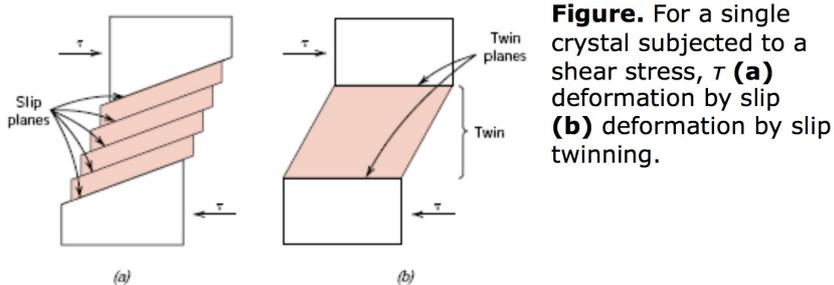
$$\sigma_y = \frac{30 \text{ MPa}}{(\cos 45^\circ)(\cos 54.7^\circ)} = 73.4 \text{ MPa (10,600 psi)}$$



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## Twinning mechanism

- A part of the atomic lattice is deformed so that it forms a mirror image of the un-deformed lattice next to it.
- **Twinning plane**: is the plane between the un-deformed and deformed parts of the metal lattice



65



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## Comparison between slip and twinning mechanisms

slipping	twinning
1. the atoms in one side of the slip plane all move equal distances	1. the atoms move distances proportional to their distance from the twinning plane
2. Slip Leaves a series of steps (lines)	2. Twinning leaves small but well defined regions of the crystal deformed
3. Most for FCC and BCC structure, they have more slip systems	3. Is most important for HCP structure, because its small number of slip system
4. normally slip results in relatively large deformations	4. only small deformations result for twinning

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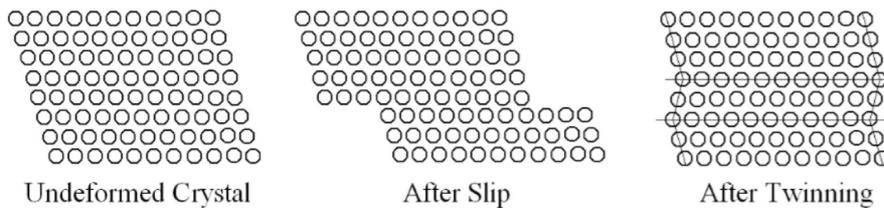
### Plastic deformation mechanisms – Twinning

- It results when a portion of crystal takes up an orientation that is related to the orientation of the rest of the untwined lattice in a definite, symmetrical way.
- The important role of twinning in plastic deformation is that it causes changes in plane orientation so that further slip can occur.
- Twinning also occurs in a definite direction on a specific plane for each crystal structure.

Crystal	Example	Twin plane	Twin direction
FCC	Ag, Au, Cu	(111)	[112]
BCC	$\alpha$ -Fe, Ta	(112)	[111]
HCP	Zn, Cd, Mg, Ti	(10 $\bar{1}2$ )	$[\bar{1}011]$ <sub>67</sub>

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### Slip Vs. Twinning



	during/in slip	during/in twinning
Crystal orientation	Same above and below the slip plane	Differ across the twin plane
Size (in terms of inter-atomic distance)	Multiples	Fractions
Occurs on	Widely spread planes	Every plane of region involved
Time required	Milli seconds	Micro seconds
Occurrence	On many slip systems simultaneously	On a particular plane for each crystal <sub>68</sub>

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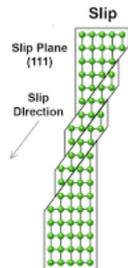
## Slip and Twin structures



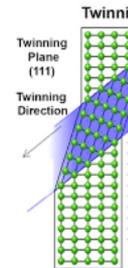
**Figure 1-3** Twin boundaries in brass.

Twin boundaries occur when two crystals mirror each other. For some materials, twinning occurs due to work hardening at low temperatures.

**Slip**



**Twinning**



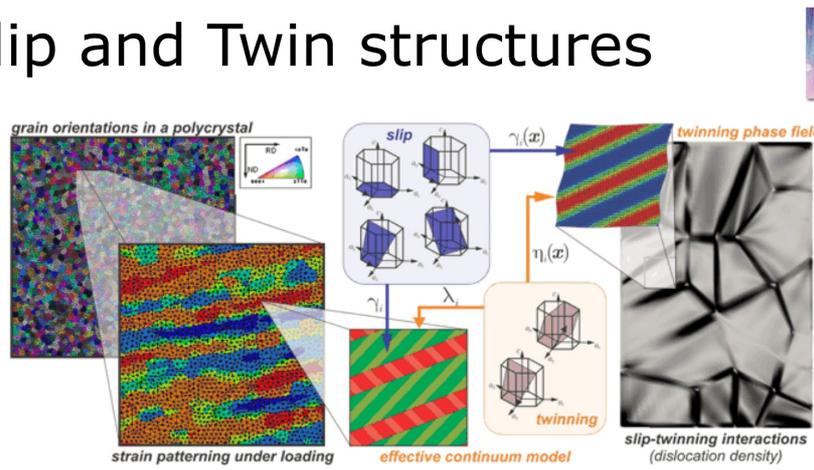
Not. To correctly determine the grain size in these types of materials, the twin boundaries need to be removed from the calculation.

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75

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## Slip and Twin structures



grain orientations in a polycrystal

strain patterning under loading

effective continuum model

slip

twinning

slip-twinning interactions (dislocation density)

$\gamma_i(x)$

$\eta_i(x)$

$\lambda_i$

$\gamma_t(x)$

twinning phase field

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## Slip and Twin structures

Fig. SEM-EBSD based slip trace analysis on Mg – 3Y:  
**HCP structure**

**Red lines** show basal slip traces  $\delta$  0001  
**Orange lines** show 1st order pyramidal slip traces 1011  
**Yellow lines** show 2nd order pyramidal slip traces 1122 ;

Secondary twins (0001)  
 (10-11) (0001)  
 (11-22) (10-11)  
 (11-20)

Legend:  
■ {0001} basal slip plane  
■ {1010} prismatic slip plane  
■ {1011} pyramidal slip plane

alpha titanium (HCP)

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## Polycrystalline Materials

*Most materials are polycrystalline and are made of many single crystals*

- during *solidification* the crystal nucleate and grow from the liquid in a *random orientation*
- the *grains* impinge on each other when the solidification is complete
- junction of grains are *grain boundaries*

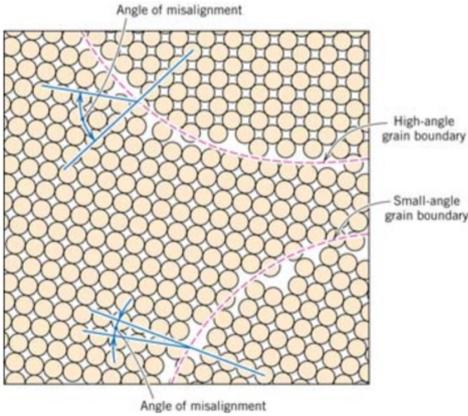
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## Grain Boundaries





- Occurs due to the crystallographic mismatch when two grains meet
- when mis-orientation is large → **high angle grain boundary**
- when mis-orientation is small, → **low angle grain boundary**
- atoms are **less bonded** and the atomic packing is lower than in the grain (*lower coordination*)
- the result is an energy difference → *interfacial surface energy or grain boundary energy*

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