HOMEWORK
From Dieter
4-6

Module #8

Defects in Crystalline Materials

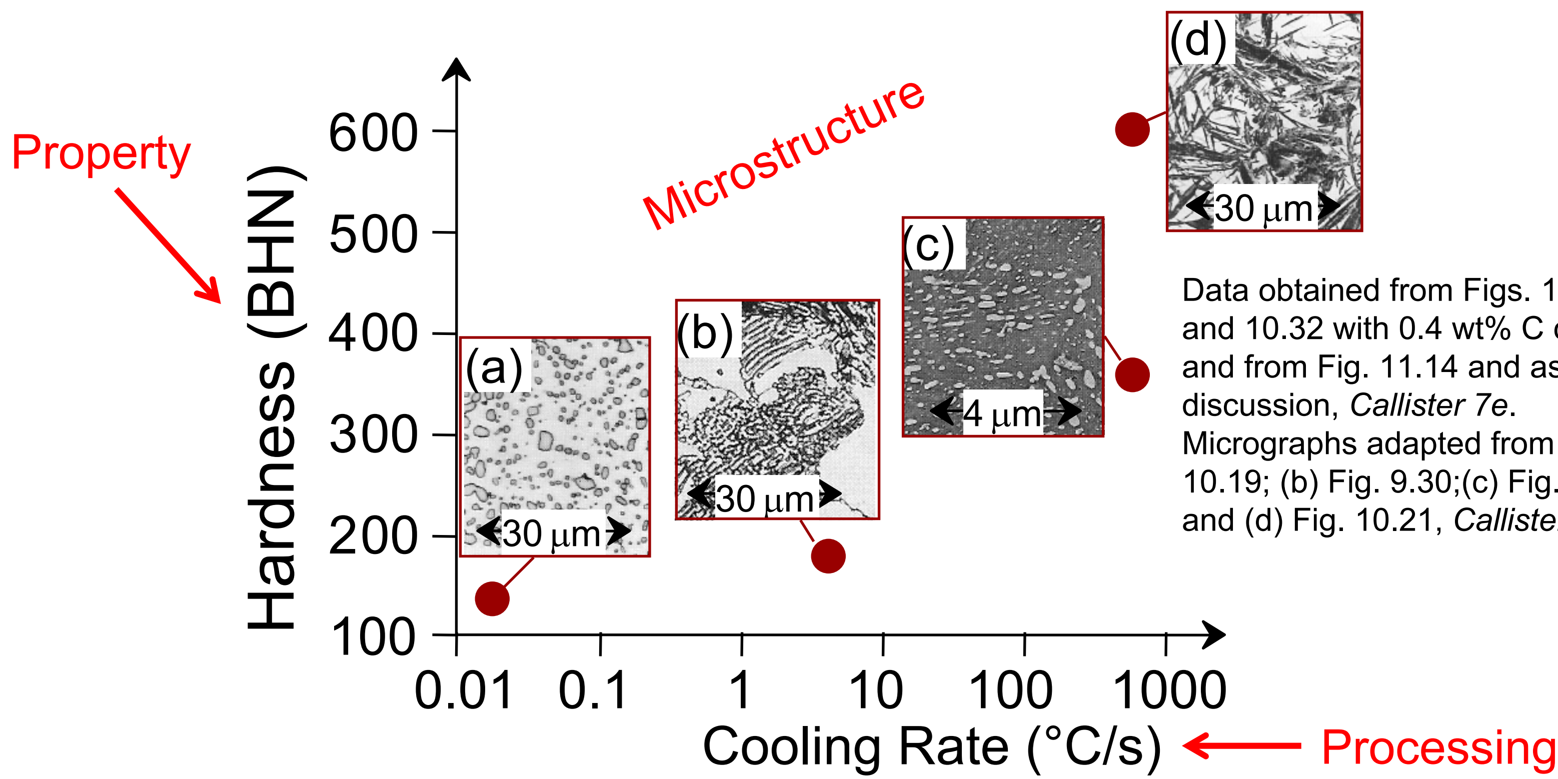
READING LIST

DIETER: Ch. 4, Pages 103-114

Ch. 4, Pages 103-117 in Meyers & Chawla, 1st ed.
Ch. 1, Pages 1-26 in Argon

Structure, Processing, & Properties

- Properties depend on structure
  ex: hardness vs. structure of steel



Data obtained from Figs. 10.30(a) and 10.32 with 0.4 wt% C composition, and from Fig. 11.14 and associated discussion, *Callister 7e*. Micrographs adapted from (a) Fig. 10.19; (b) Fig. 9.30;(c) Fig. 10.33; and (d) Fig. 10.21, *Callister 7e*.

- Processing can change structure
  ex: structure vs. cooling rate of steel

Crystals

FCC

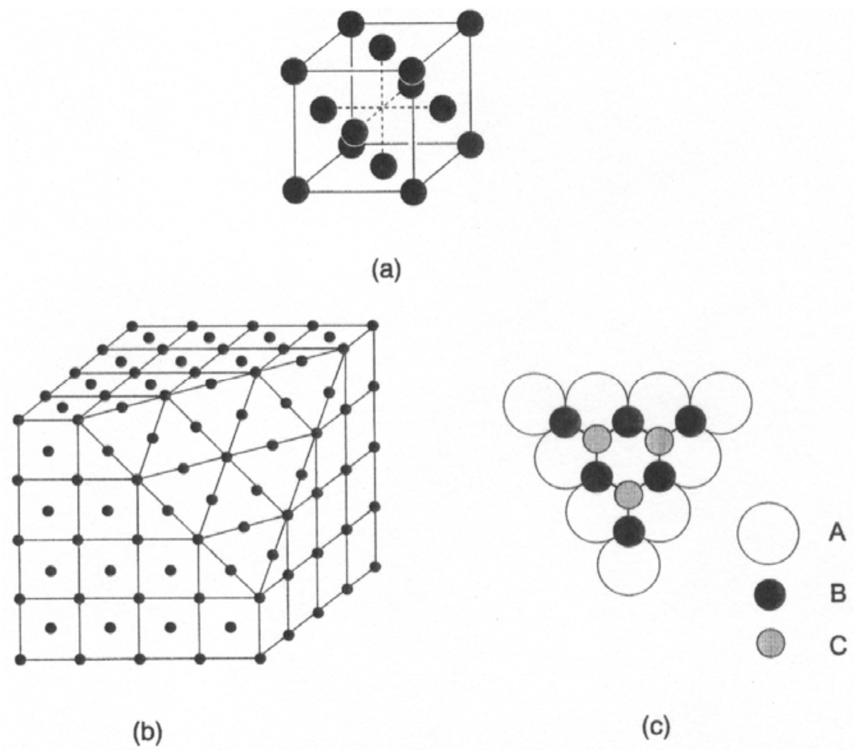


Fig. 1.7 from Hull & Bacon, 4th ed.

HCP

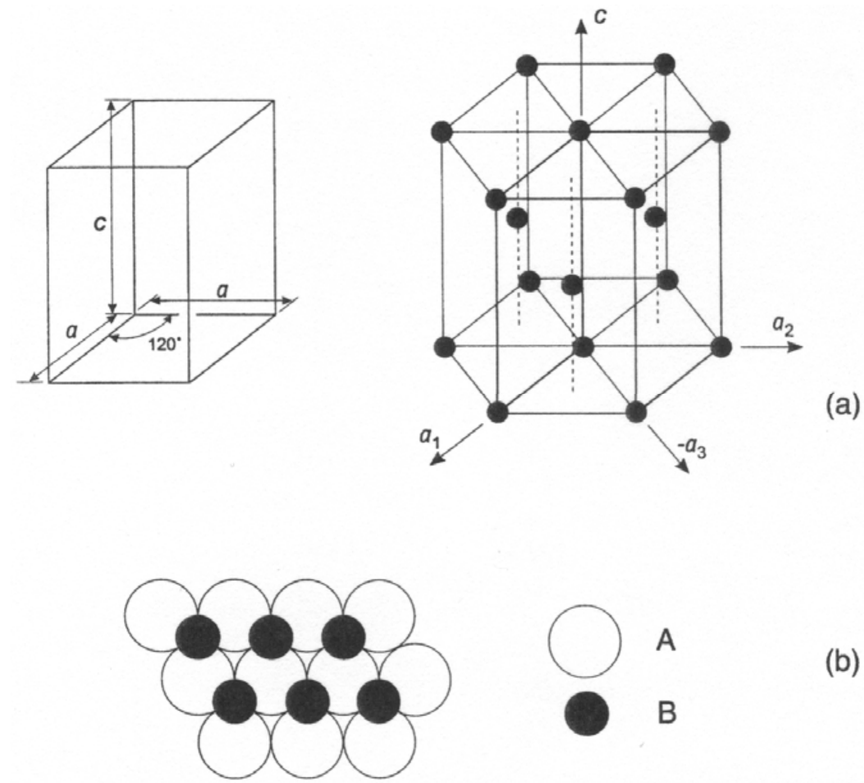


Fig. 1.8 from Hull & Bacon, 4th ed.

Solids where atoms, ions, or molecules occupy specific lattice sites and exhibit specific symmetry relationships in their arrangement.

Lattice Defects

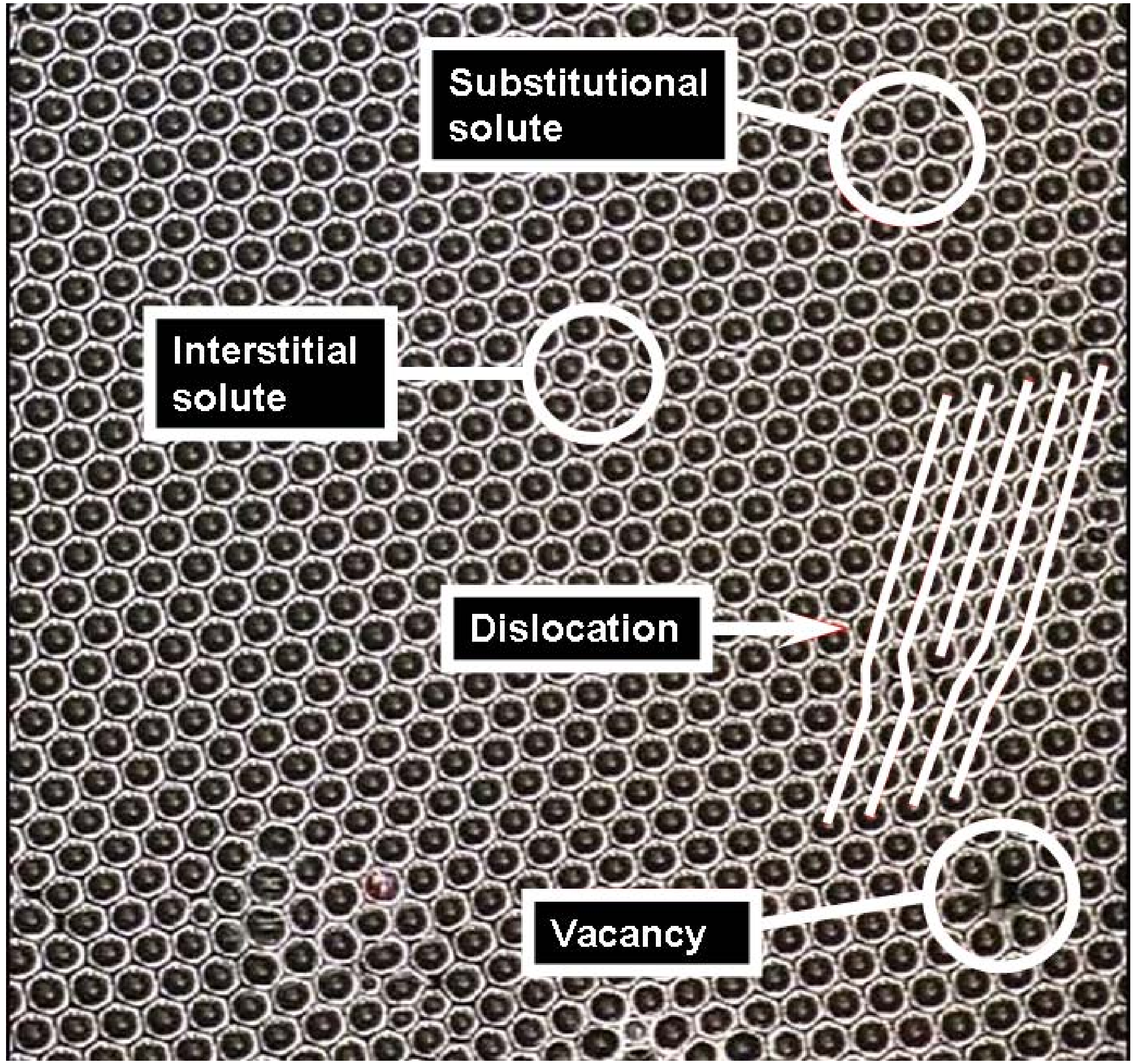
► Real crystals do not exhibit perfect periodicity.

- Lattice defects describe any variation from a periodic array of lattice points.

Structure-insensitive	Structure-sensitive
Elastic constants	Electrical conductivity
Melting point	Semiconductor properties
Density	Yield stress
Specific heat	Fracture strength
Coefficient of thermal expansion	Creep strength

- Lattice defects and their interactions determine structure-sensitive properties.

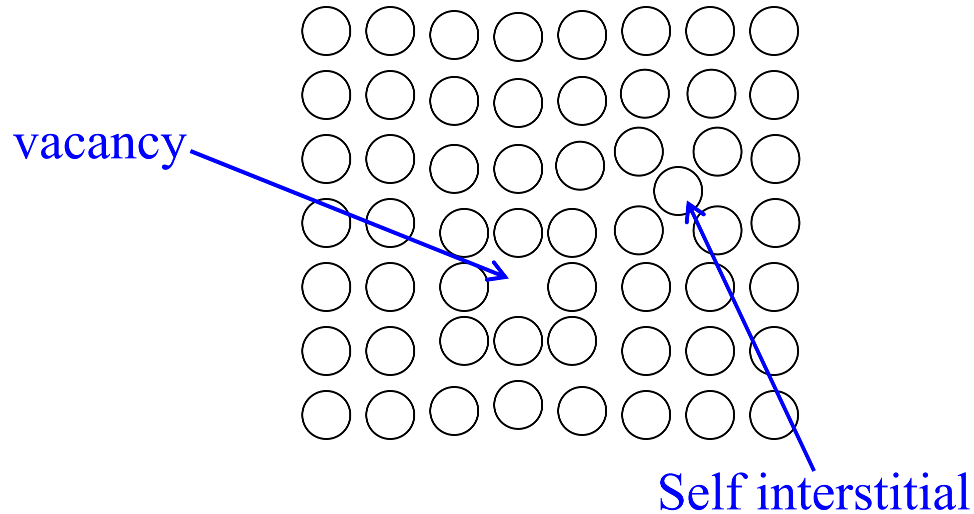
- Point Defects (0-D)
- Line Defects (1-D)
- Planar Defects (2-D)
- Volume Defects (3-D)



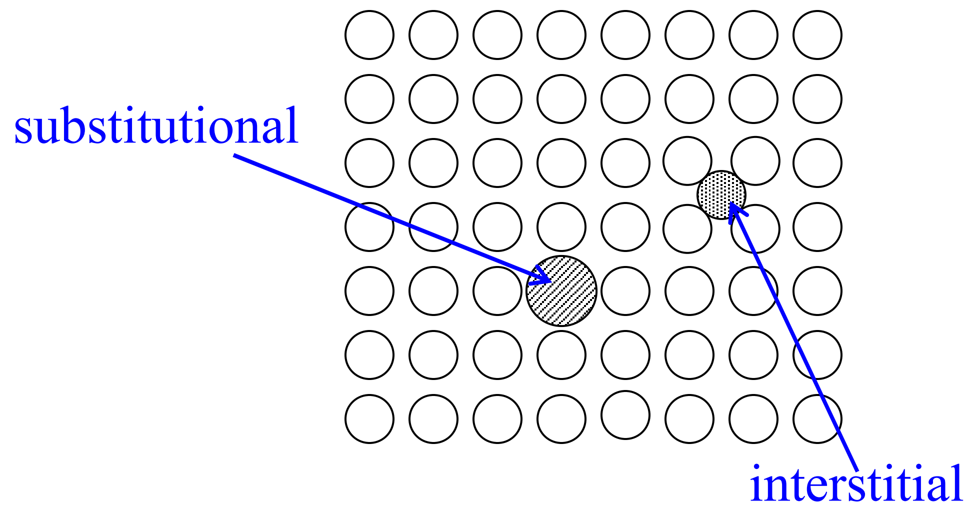
http://www.msm.cam.ac.uk/doitpoms/tlplib/dislocations/images/raft3.jpg

Point Defects (0-D)
(metals or elemental semiconductors)

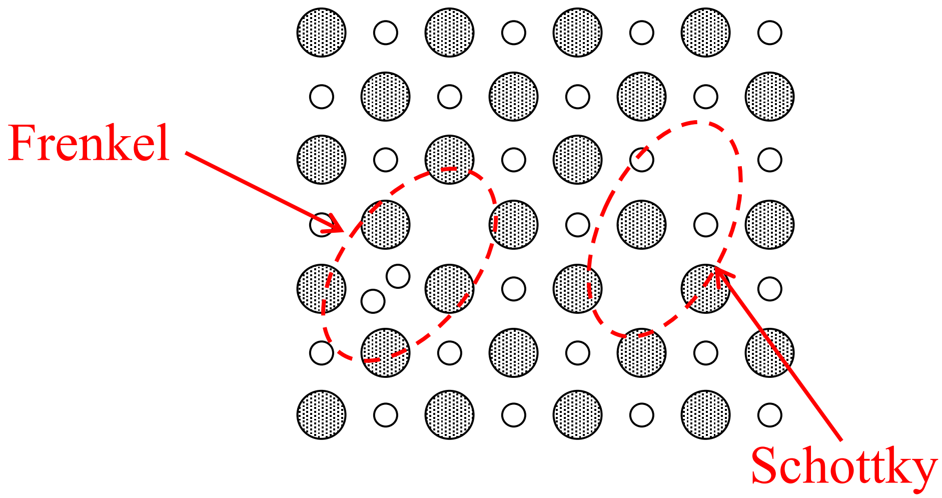
Vacancy and interstitial point defects



Impurities: substitutional and interstitial point defects



Other Point Defects
(compound structures – ceramics and ionic crystals)



Schottky Defect

a pair of oppositely charged ion vacancies

Frenkel Defect

vacancy–interstitial combination

Vacancies and Interstitials

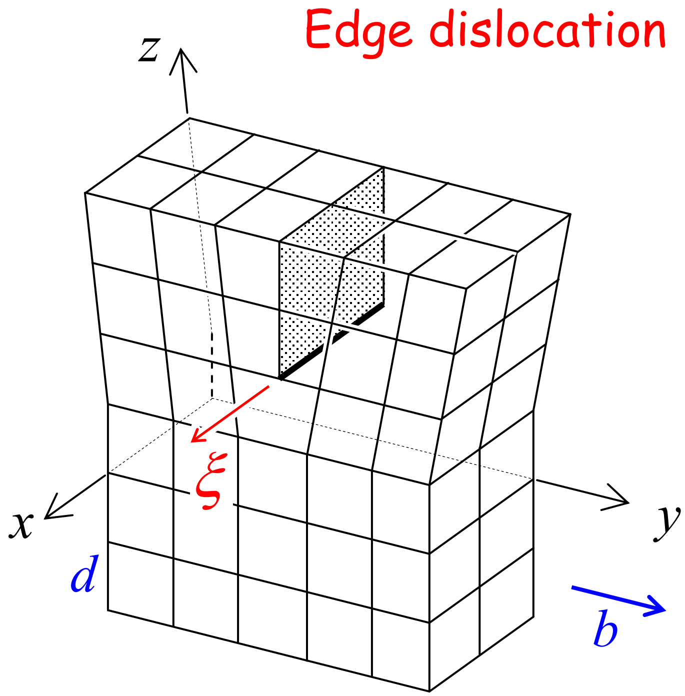
- At low temperatures, diffusional processes are too slow to be of importance in deformation.
- Point defects can play a supporting role in dislocation based plasticity.
- Point defects distort the crystal lattice.
- At high temperatures, where diffusion is significant, point defects can play a significant role in plasticity.

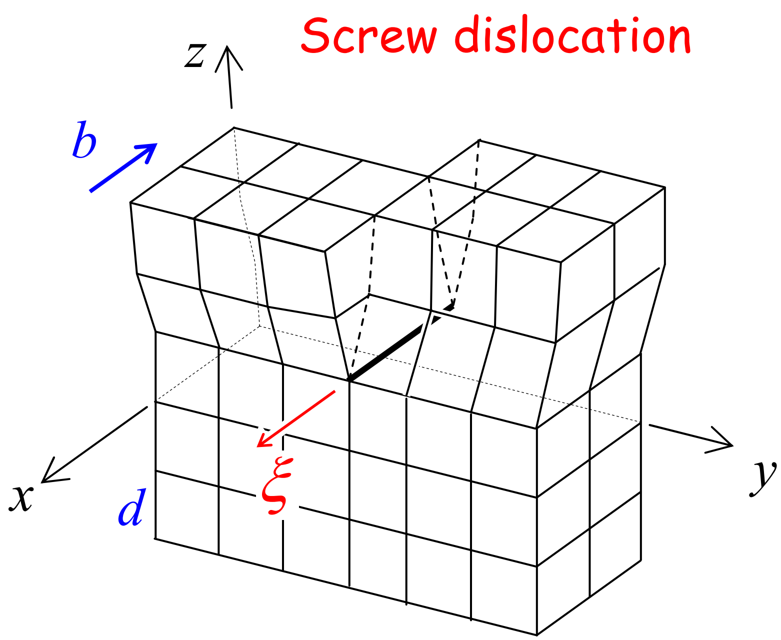
Point Defects (0-D)

- Production/Sources
  - Quenching
  - Irradiation
  - Ion implantation

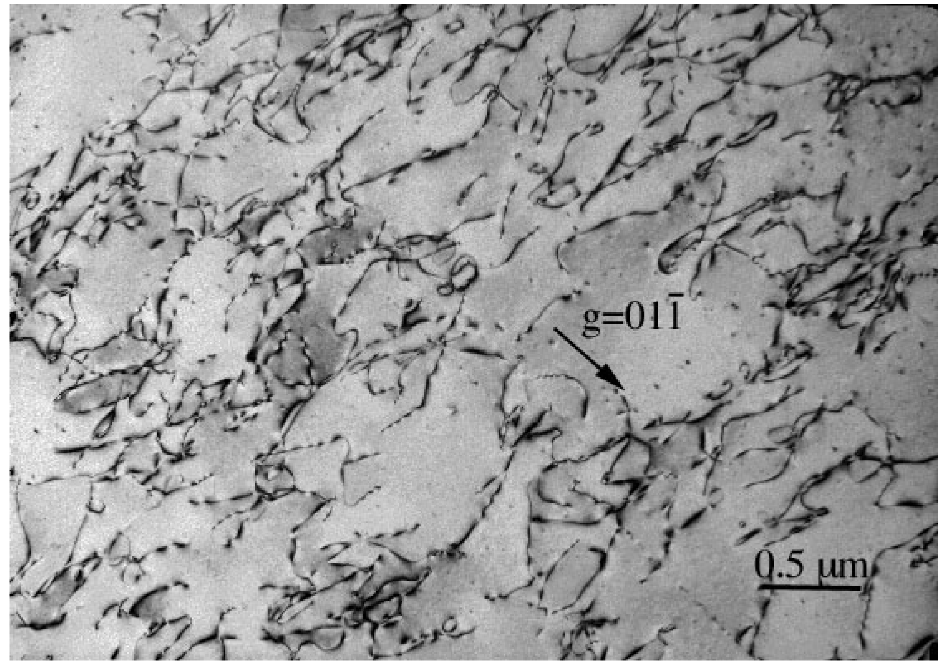
- Influence on Mechanical Properties
  - Aid plastic deformation via diffusion
  - Increased yield strength when interact w/ line defects
  - Can also cause embrittlement

Line Defects (1-D)





Dislocations



[Weaver, 1995]

Linear defects around which atoms are "dislocated" from their equilibrium lattice positions.

Line Defects (1-D)

- Production/Sources
  - Crystal growth
  - Deformation

- Influence on Mechanical Properties
  - Motion leads to plastic deformation via shear
  - Increased yield strength when line defects interact w/ other line defects

Planar Defects (2-D)

- Grain boundaries
  - Low angle
  - High angle
  - Special (e.g., coincident site lattice, Σ5, etc…)

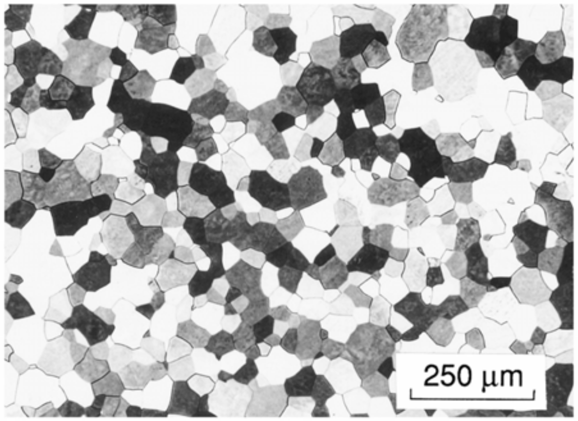
- Twin boundaries
  - Annealing
  - Deformation

- Stacking Faults
  - Intrinsic
  - Extrinsic

All of them disrupt the periodicity of the crystal lattice.
All induce strain fields!

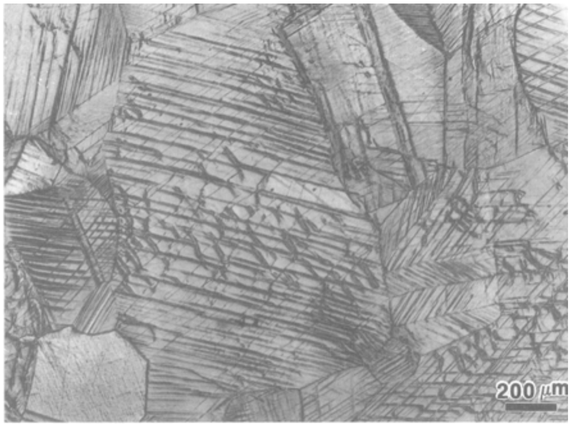
Examples of planar (2-D) defects

GRAIN BOUNDARIES



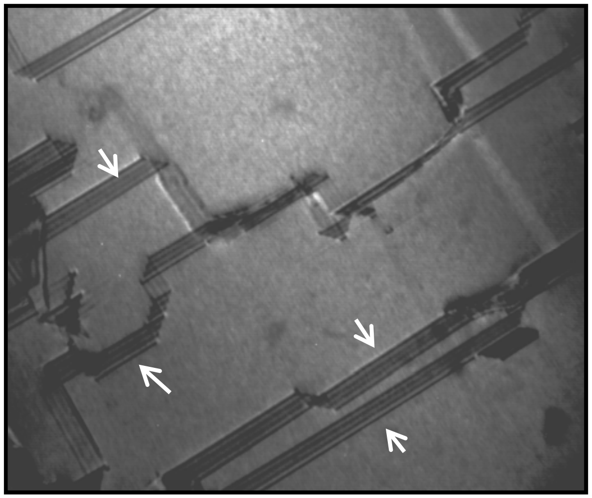
[Dowling, p.32]

DEFORMATION TWINS

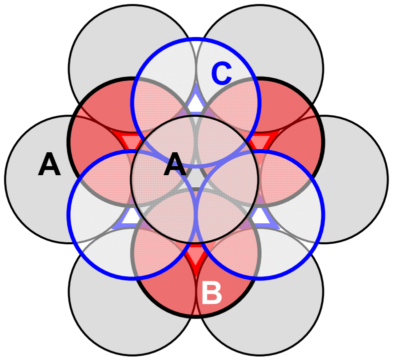


[Meyers, p.424]

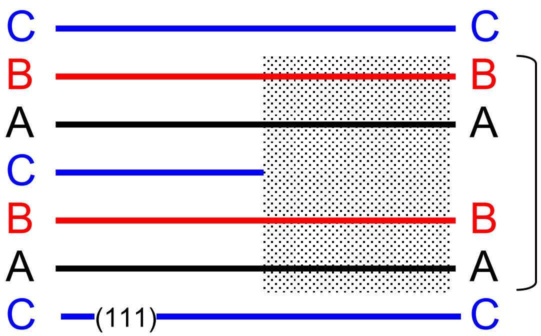
STACKING FAULTS



[Weaver, 1992]



FCC stacking sequence



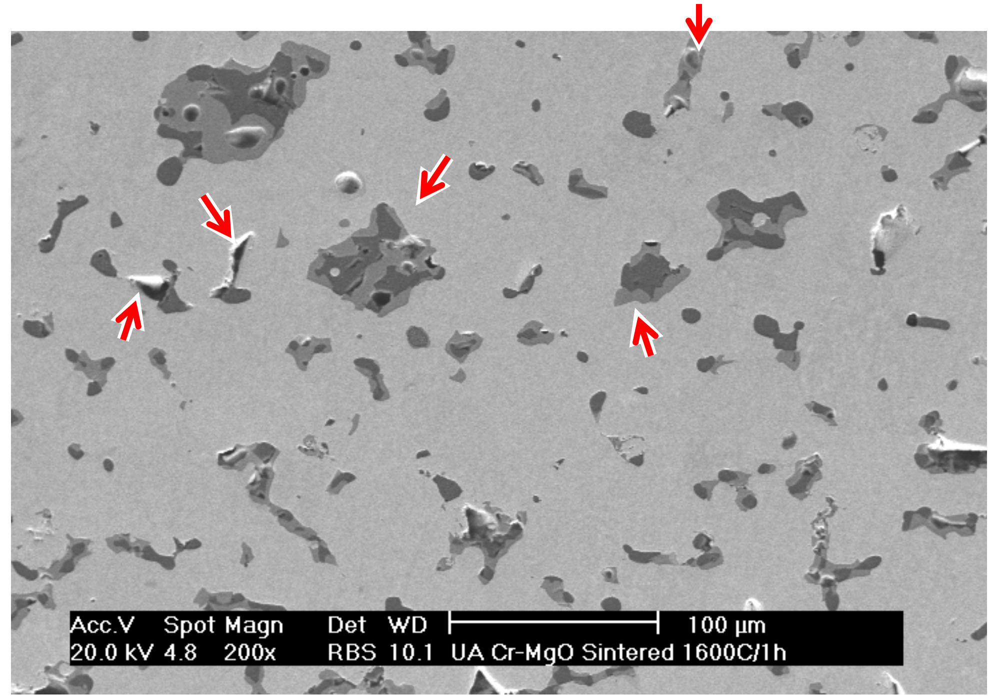
Planar Defects (2-D)

- Production/Sources
  - Crystal growth
  - Deformation
  - Annealing

- Influence on Mechanical Properties
  - Increased yield strength when interact w/ line defects

Volume Defects (3-D)

- Inclusions
  - Ex., MnS in steel
- Dispersed Particles
  - Ex., Al_2O_3 in Al
- Precipitates
  - Coherent
  - Partially coherent
  - Incoherent
- Voids



Some of them disrupt the periodicity of the crystal lattice.
Some induce strain fields!

Volume Defects (3-D)

- Production/Sources
  - Solidification and heat treatment of certain alloys
  - Phase transition
  - Other processing methods

- Influence on Mechanical Properties
  - Increased yield strength when interact w/ line defects
  - Can improve or reduce resistance to diffusive flow
  - Etc…

Line Defects (1-D) Dislocations

- In the rest of this course, dislocations will be directly or indirectly involved with all of the topics that we discuss.
- A dislocation is a line that forms a boundary between a region of a crystal that has slipped and one that has not.

Volterra 1907

- Considered rotational and translational dislocations.
  - Rotational dislocations are called “disclinations.”
  - Translational dislocations are called “dislocations.”
- Strength of “dislocation” is determined by its Burgers vector b.
- Strength of “disclination” is determined by its Frank vector Ω.

Volterra Dislocations and Disclinations

DISLOCATION

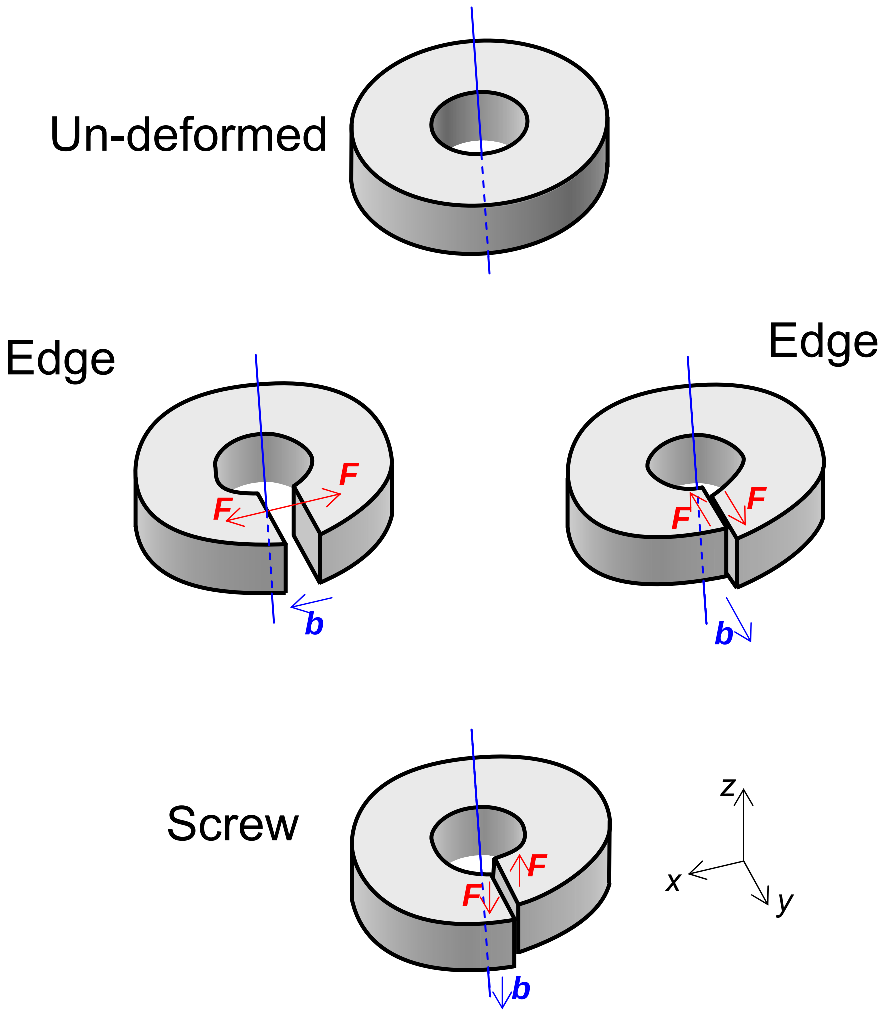


Fig. 5.10

DISCLINATION

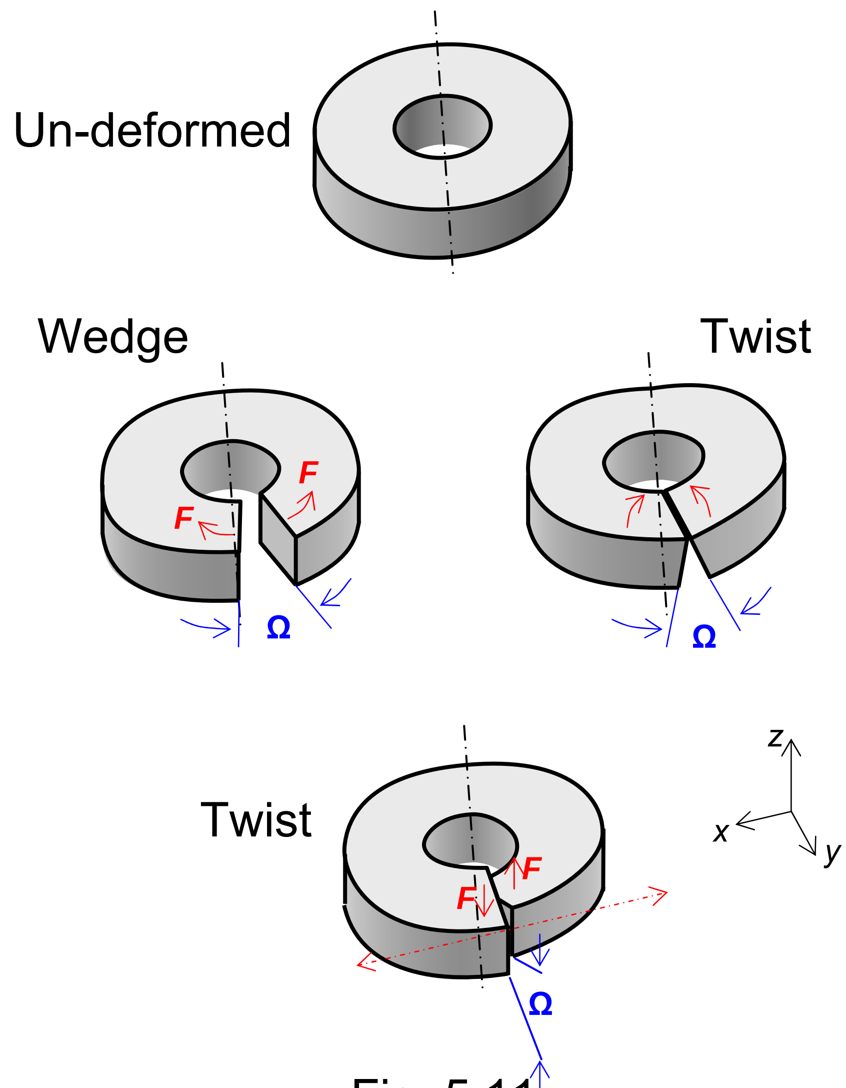


Fig. 5.11

Adapted from S.M. Allen and E.L. Thomas, The Structure of Materials, John Wiley & Sons (1999).

Line Defects (1-D) in Crystals

Dislocations

- Primary line defects in solid crystals.
- Involve translation of one portion of a crystal with respect to another part.

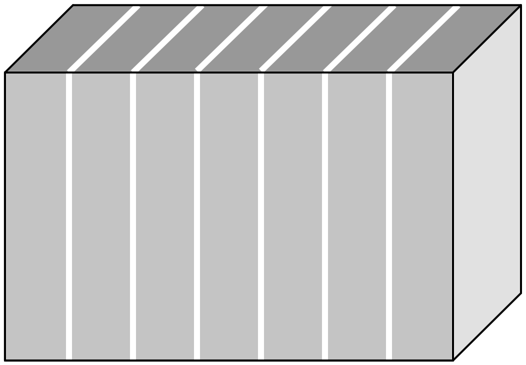
Disclinations

- Primary line defect in liquid crystals.
- Involve rotation of one part of a crystal relative to another part

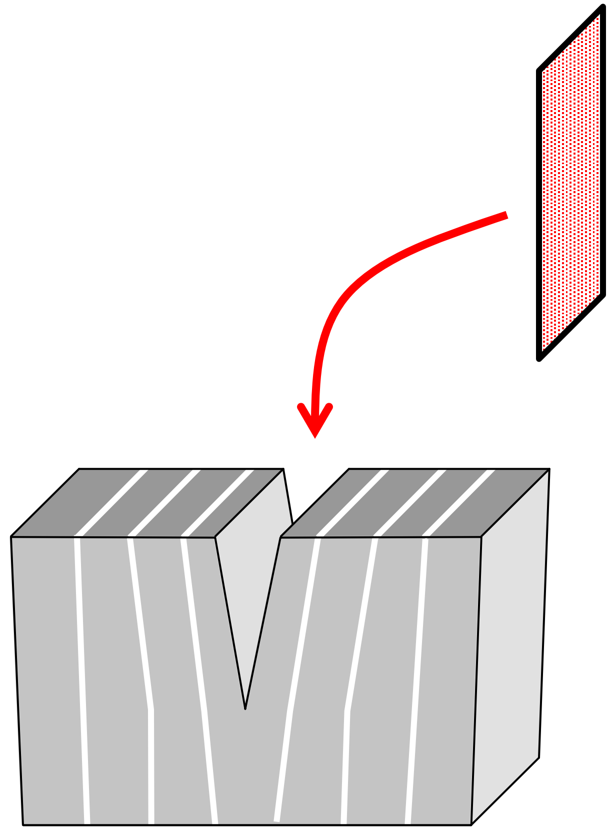
From this point forward we shall refer to translational dislocations simply as "dislocations"

Basic Types of Dislocations

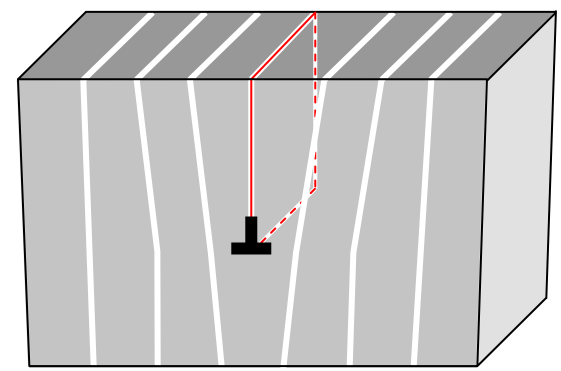
- Edge
- Screw



Perfect crystal

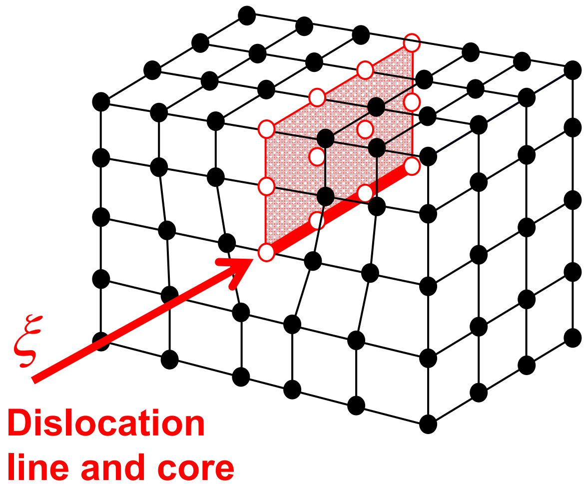


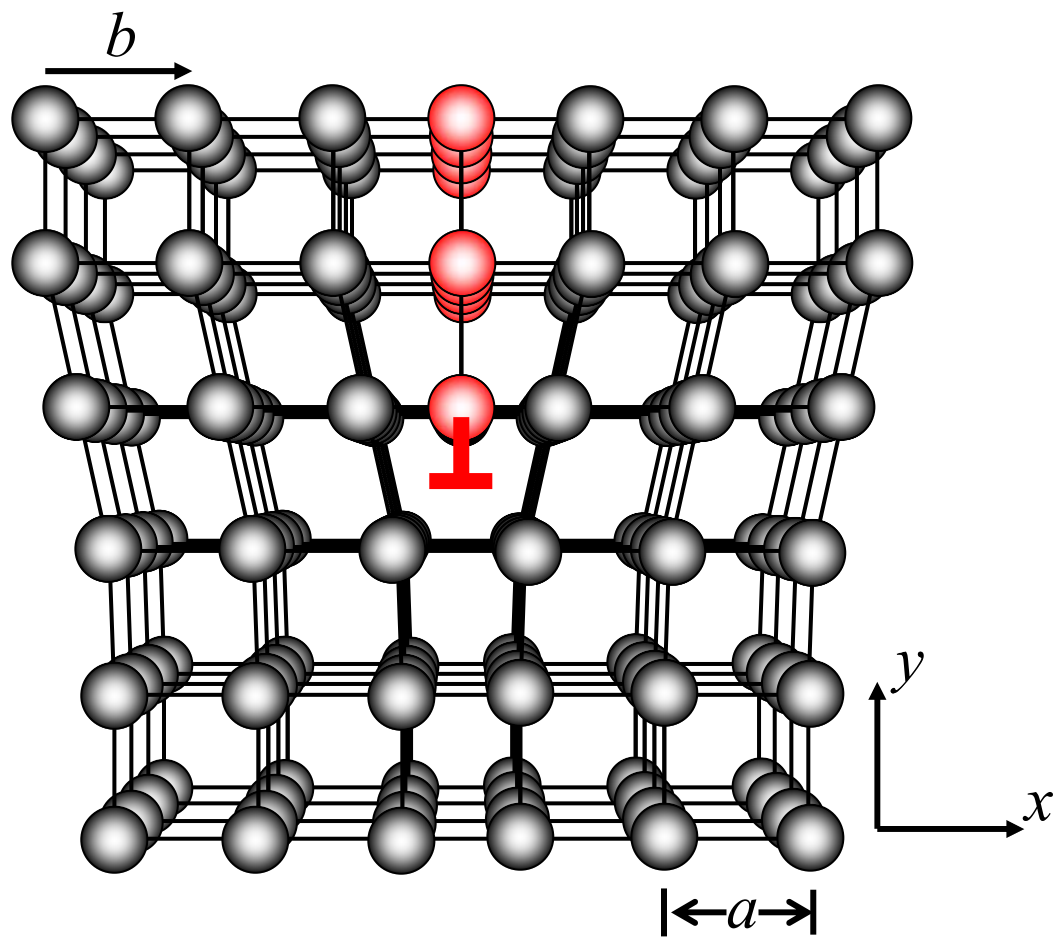
Split to center
& insert extra ½ plane of
atoms



EDGE DISLOCATION

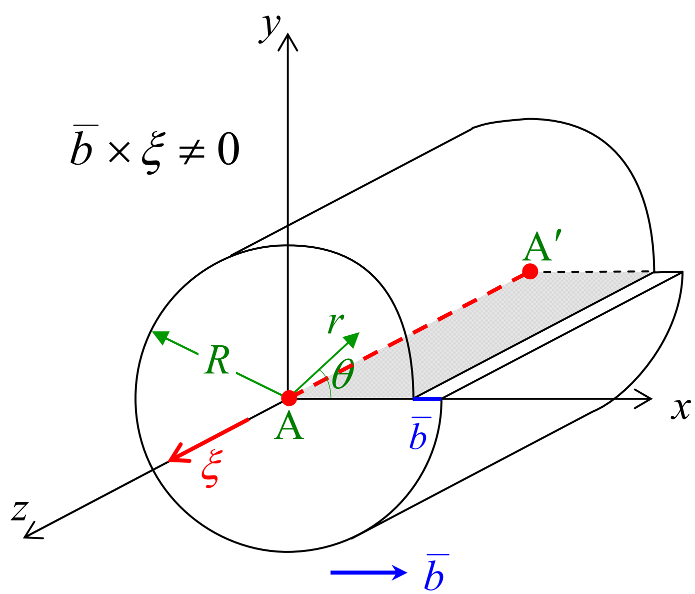
Atomic Scale Visualization of an EDGE DISLOCATION





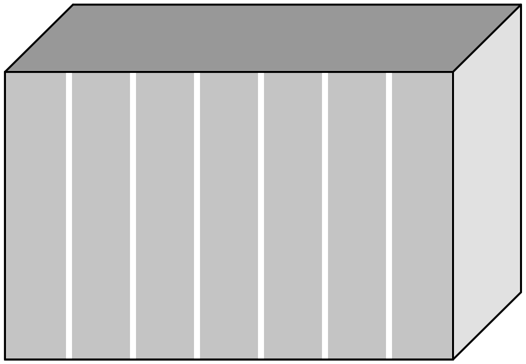
NOTE : $\ell, \xi,$ and $\hat{t}$ are often used to indicate the dislocation line direction (i.e., the "sense" vector).

Edge Dislocation

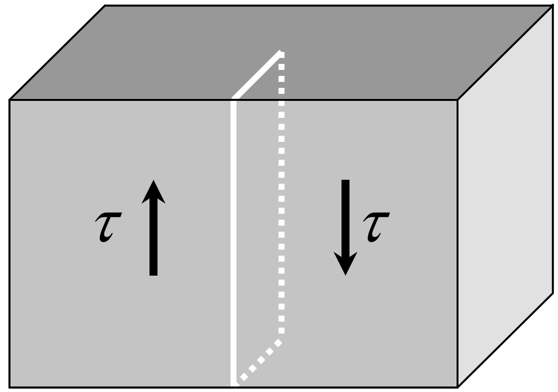


Geometries of an edge dislocations in an elastic cylinder.

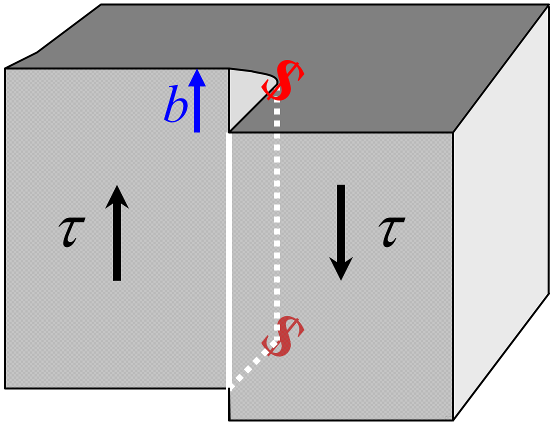
[Figure adapted from A.S. Argon, Strengthening Mechanisms in Crystal Plasticity, (Oxford University Press, Oxford, 2008) p. 17]



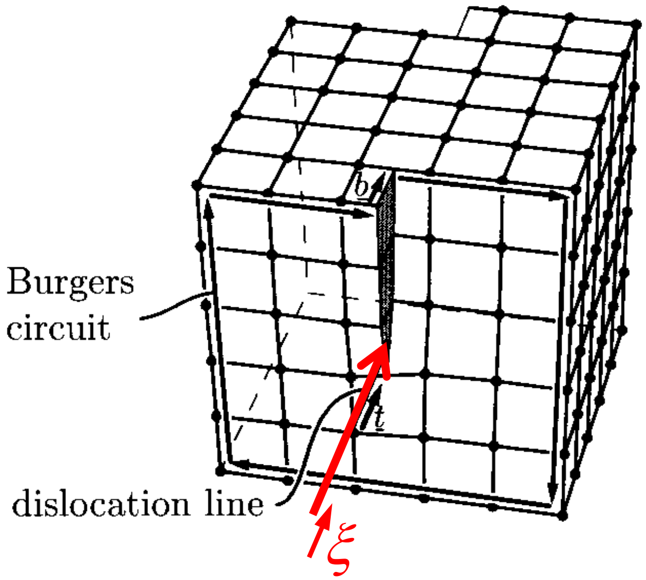
Perfect crystal



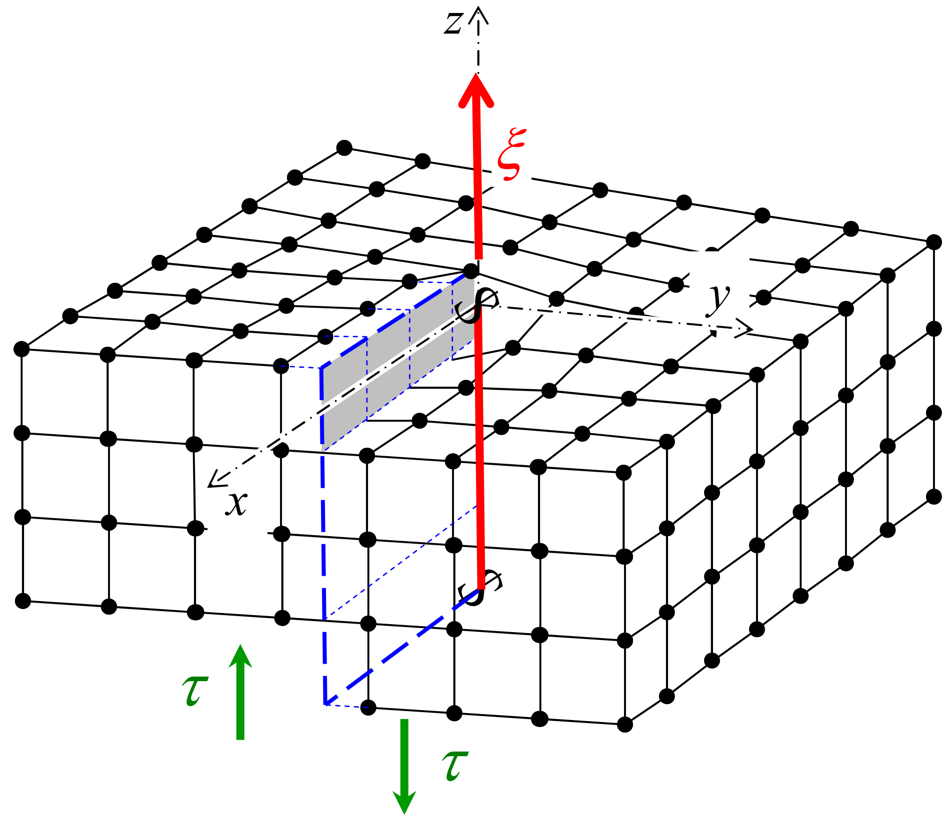
Split to center and
slide cut faces across each other
(*i.e. shear them)*



SCREW DISLOCATION



[Roesler, p.167]



[Adapted from McClintock, p.198]

Some Common Symbols : $

Atomic Scale Visualization of a

SCREW DISLOCATION

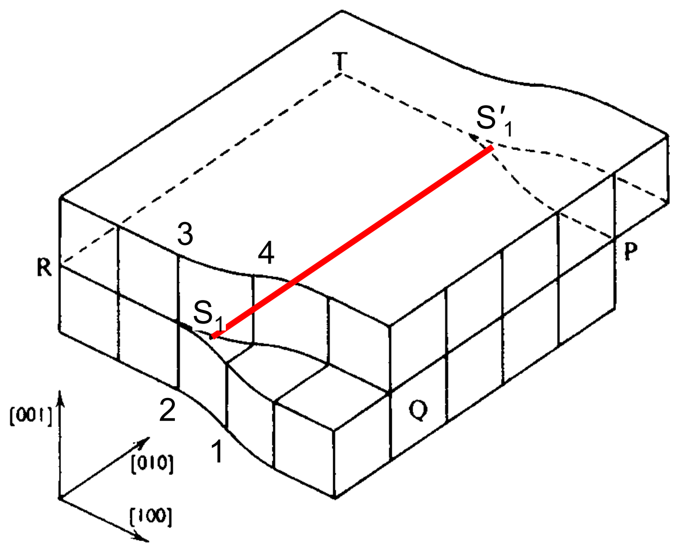


Figure 7.1 A screw dislocation in a primitive cubic lattice

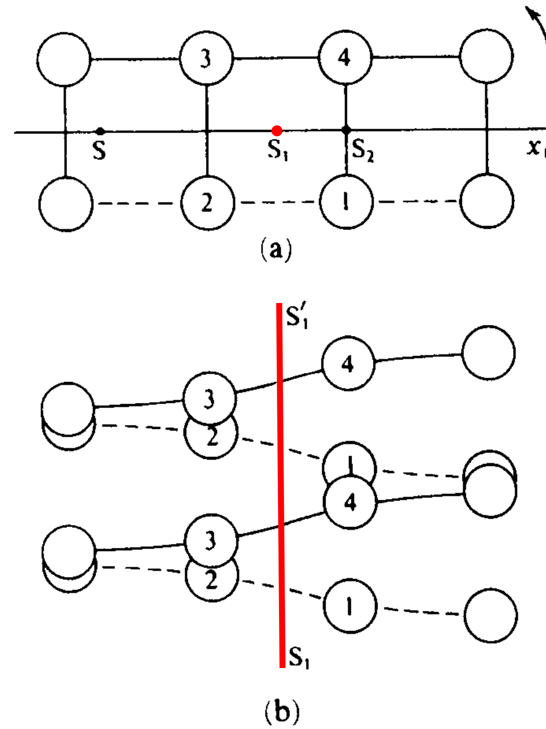
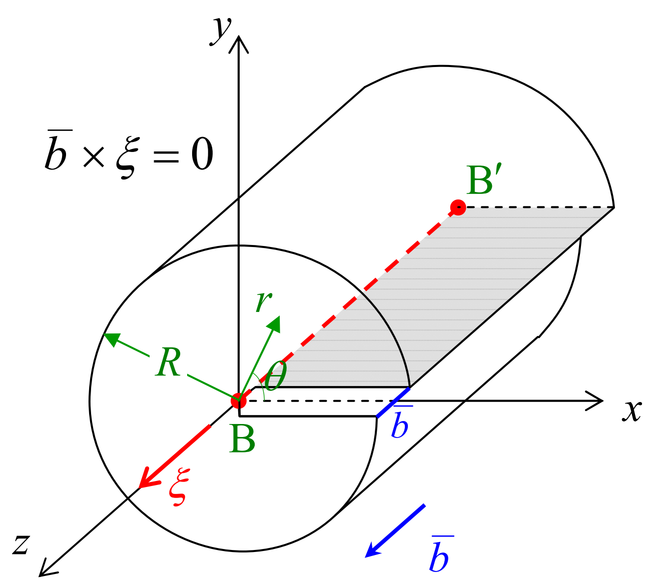


Figure 7.6 Screw dislocation in a simple cubic crystal (a) looking along the dislocation and (b) looking normal to the dislocation which lies along $S_1S'_1$.

Adapted from Kelly, Groves and Kidd, *Crystallography and Crystal Defects, Revised Edition*, John Wiley & Sons, 2000

Screw Dislocation



Geometries of a screw dislocations in an elastic cylinder.

[Figure adapted from A.S. Argon, Strengthening Mechanisms in Crystal Plasticity, (Oxford University Press, Oxford, 2008) p. 17]

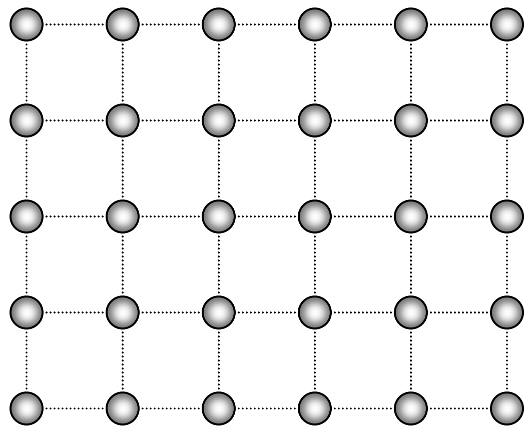
The dislocation type (i.e., character) depends upon the relationship between the *Burgers vector* (b) and the *dislocation line* (ξ)

How to establish the character?

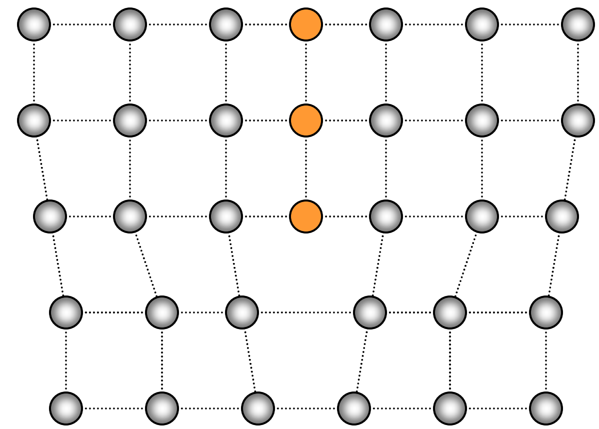
"Draw a Burgers circuit"

Look at angle between the Burgers vector and the dislocation line.

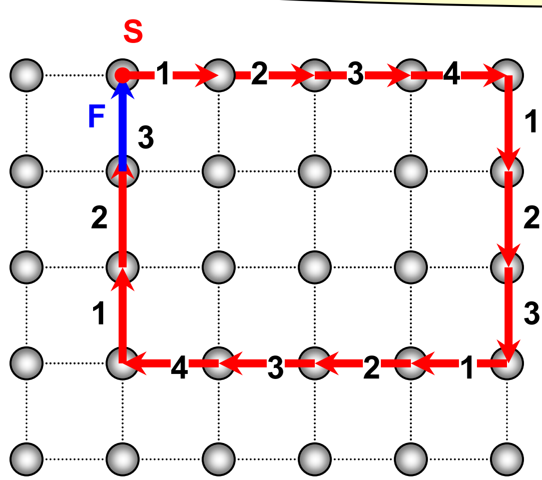
PERFECT LATTICE



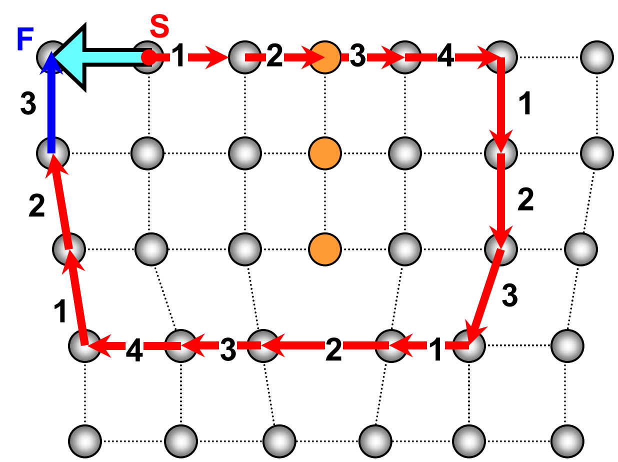
"DISLOCATED" LATTICE



sketch *m* X *n* step loops of same size through both crystals

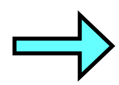


Complete closure of circuit



ξ goes into page

[**SF**/*RH*]

 = **BURGERS VECTOR**

The Burgers vectors for given dislocations <u>never</u> change!

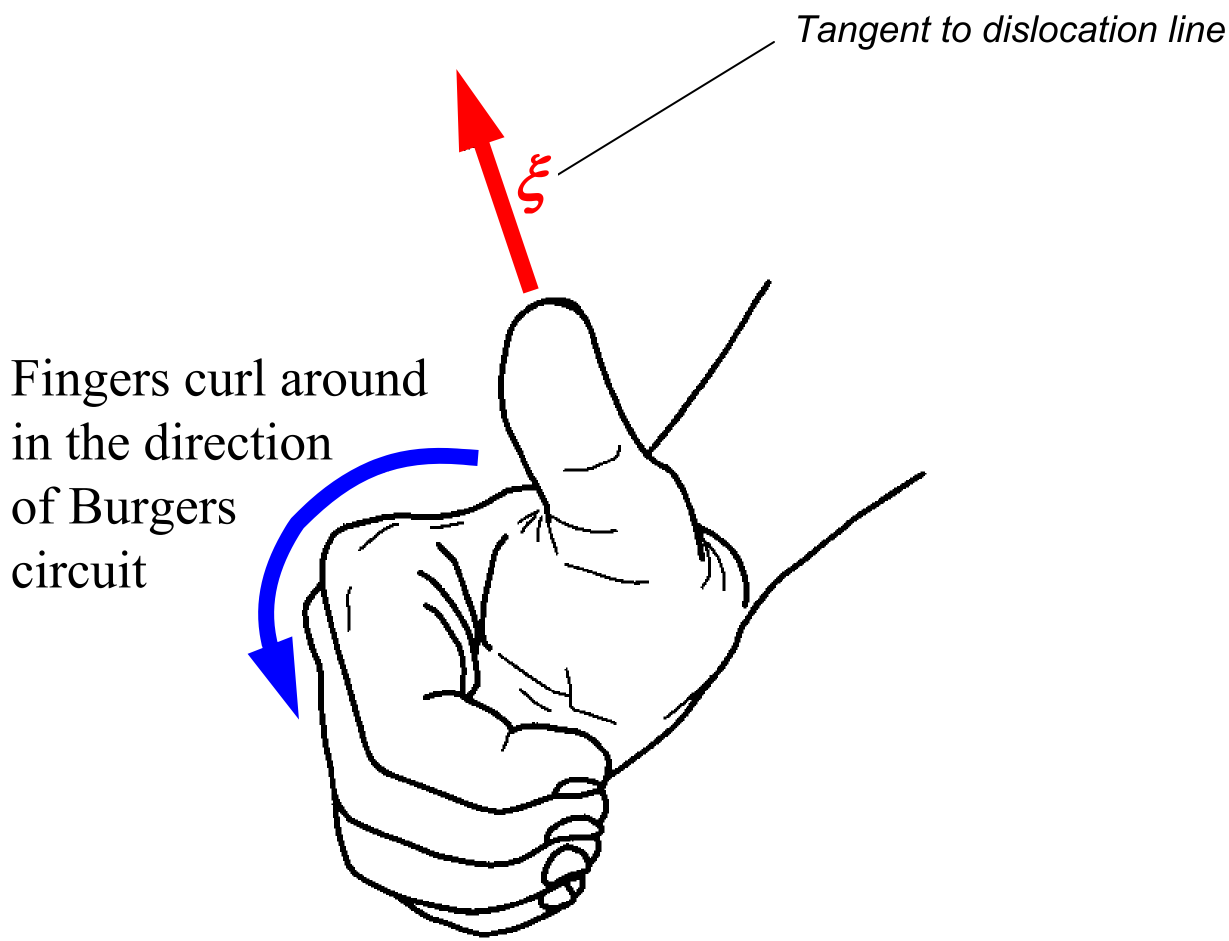


Fig. 6.3. Right-hand rule for determining the direction of a Burgers circuit. [Figure adapted from Roesler et al., p. 168]

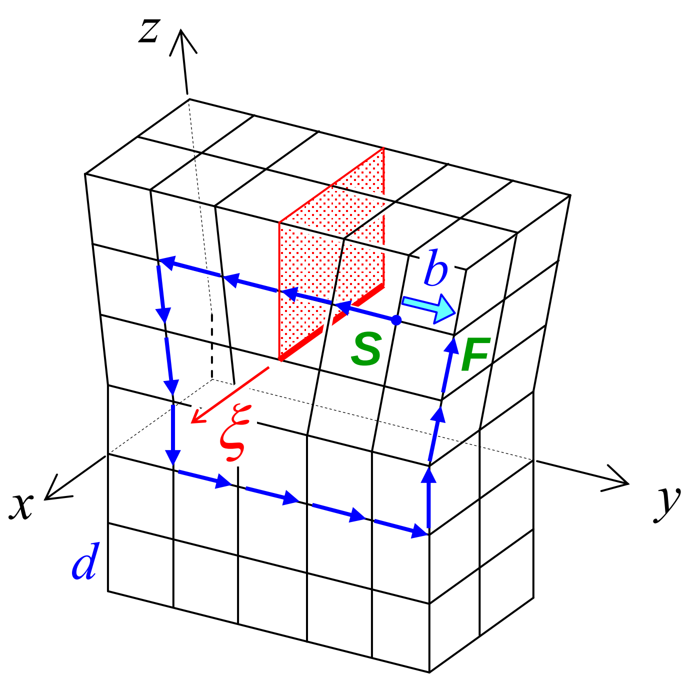


Figure 5.18 Determination of the Burgers vector of an **edge dislocation** in a simple cubic crystal. A right-handed circuit that would be closed in a perfect crystal is made surrounding the dislocation core, from starting point ***S*** to finishing point ***F***. Burgers vector ***b*** and ξ are perpendicular.

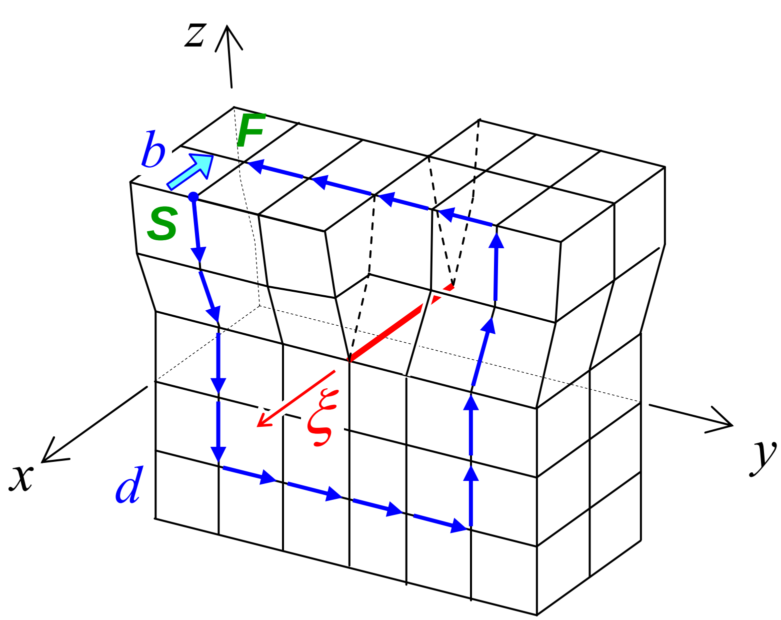


Figure 5.19 Determination of the Burgers vector of a **screw dislocation** using the **SF**/*RH* convention. For a screw dislocation, ***b*** and ξ are either parallel or antiparallel. This particular dislocation is a left-handed screw dislocation.

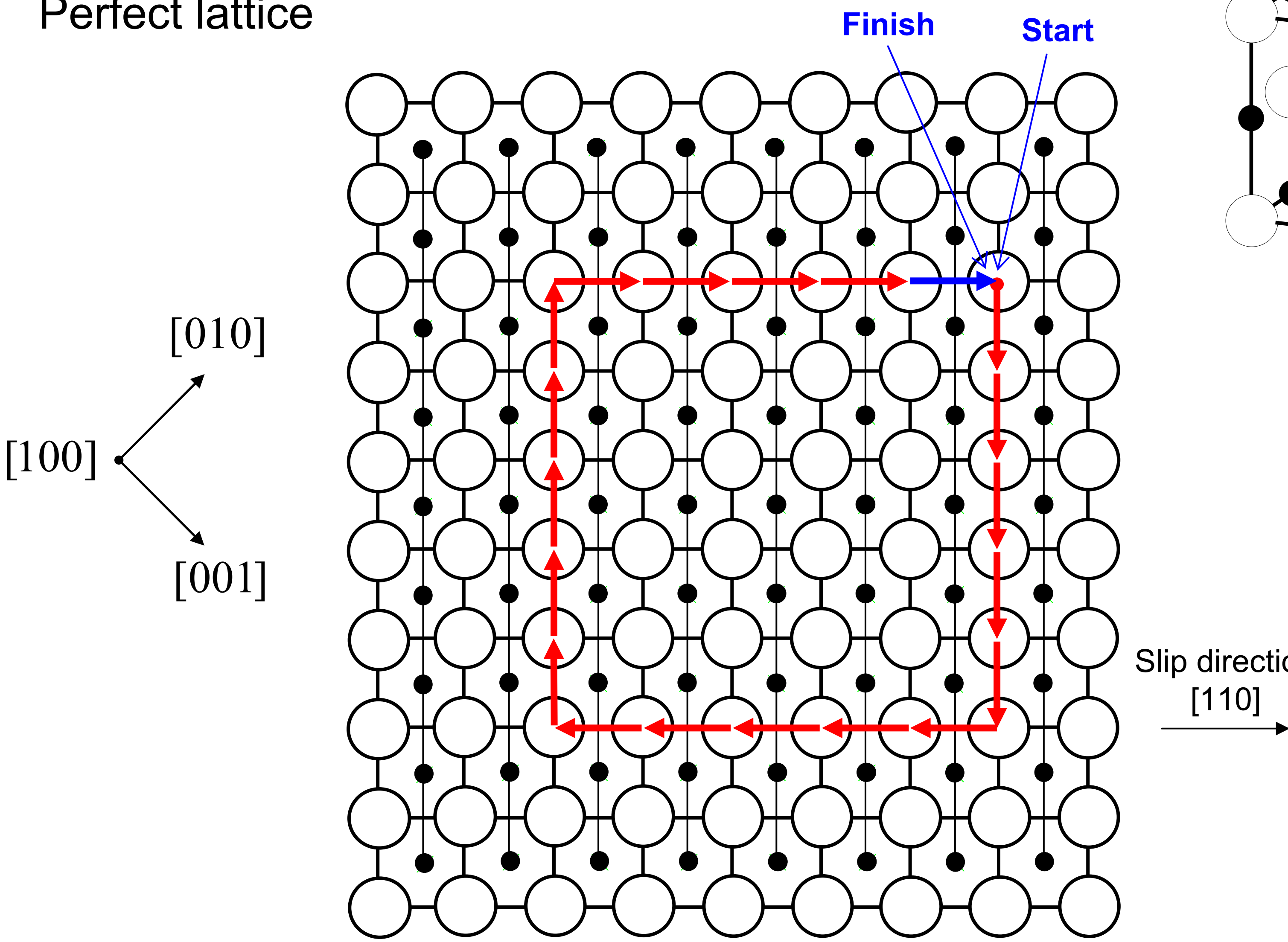
[Figures adapted from Allen & Thomas]

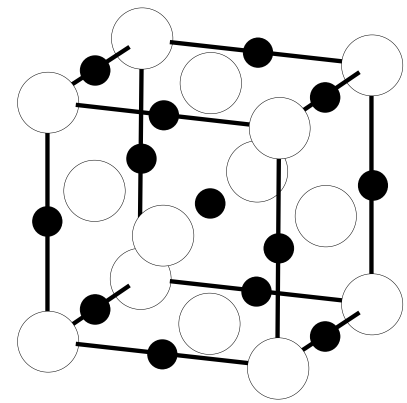
In ceramics or ionic crystals the character of a dislocation is decided the same way.

Must consider balance of charge.

Examples of edge dislocations are shown on the next two viewgraphs.

Consider MgO
Perfect lattice

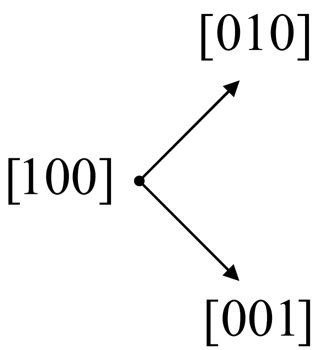


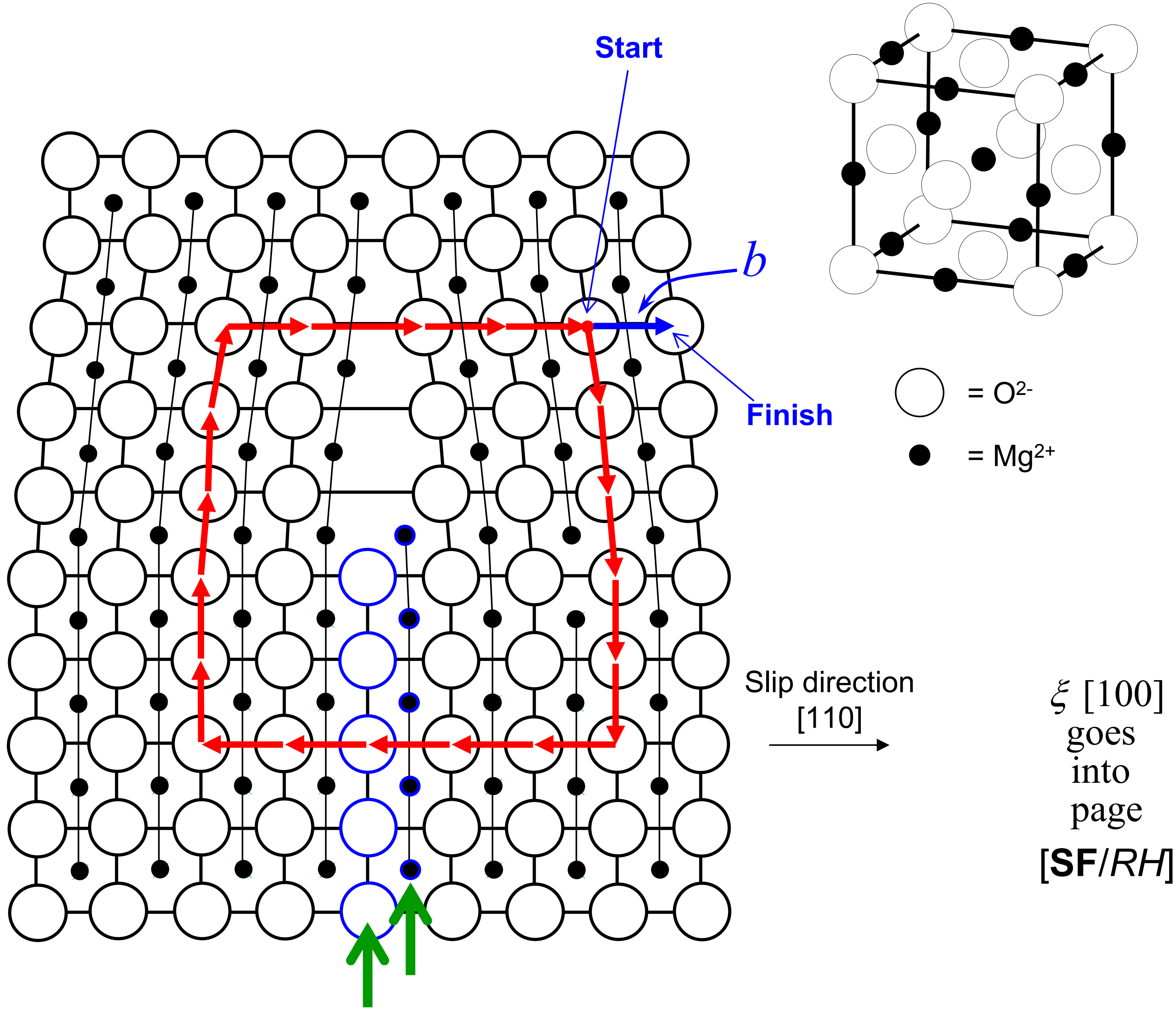


ξ [100] goes into page

[**SF**/*RH*]

Consider MgO
Perfect lattice



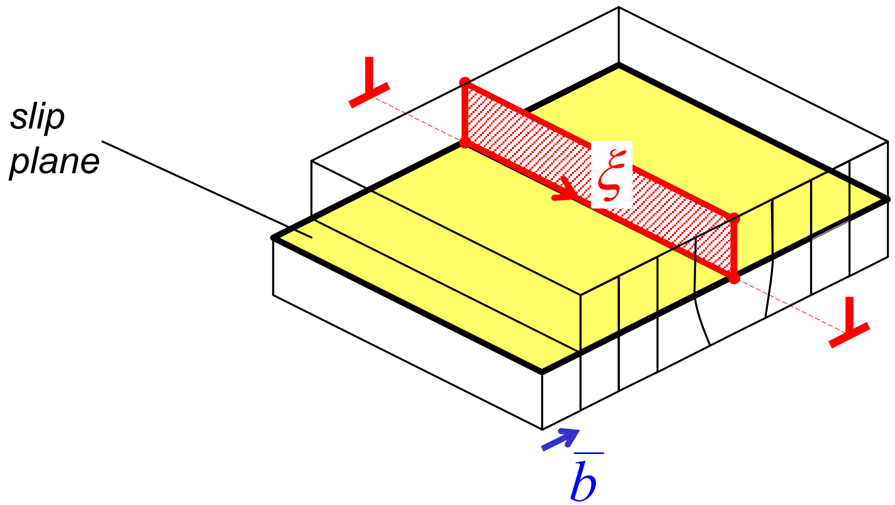


Edge dislocation in MgO showing slip direction, Burgers circuit and Burgers vector.
[Adapted from Kingery et al. Introduction to Ceramics, 2nd Edition, (Wiley, New York, 1976), p. 715]

Dislocations move on planes that contain both vector (*b*) and the dislocation line (ξ).

That plane is called the slip plane.

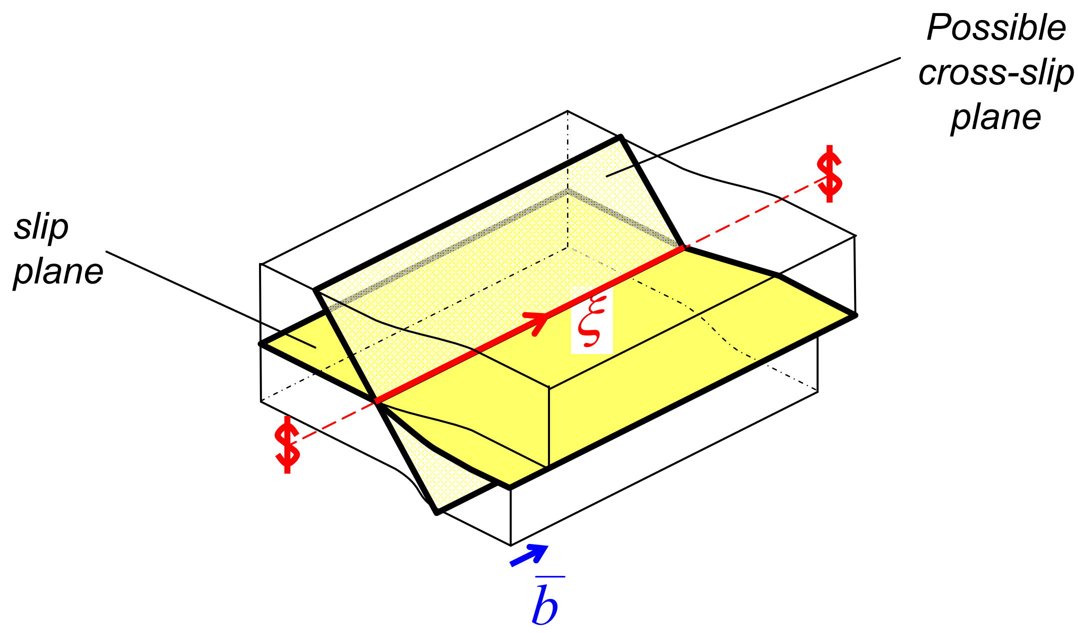
Edge Dislocation



$$\bar{b} \times \xi \neq 0$$

- The extra half plane terminates at the dislocation core.
- The Burgers vector (*b*) is perpendicular to the dislocation line (ξ).
- *b* and ξ define a ***unique slip plane*** where dislocations move.

Screw Dislocation



$$\bar{b} \times \xi = 0$$

- The Burgers vector (*b*) is parallel to the dislocation line (ξ).

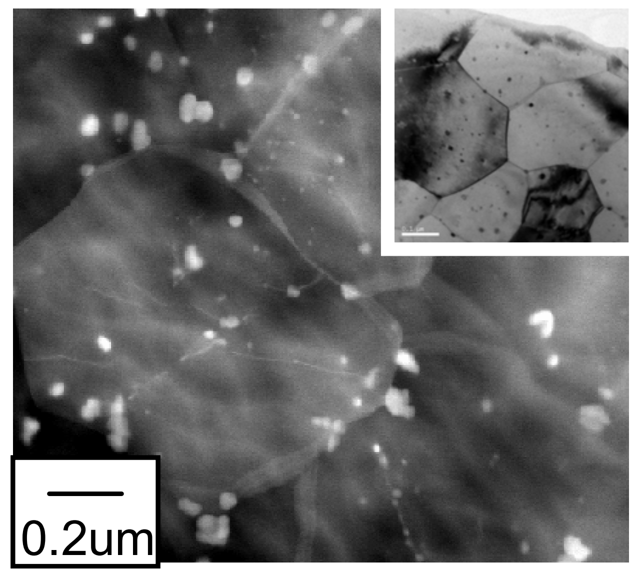
- *b* and ξ are parallel. No unique slip plane. A screw dislocation can glide on any crystallographically suitable slip plane.

Characteristics of dislocations

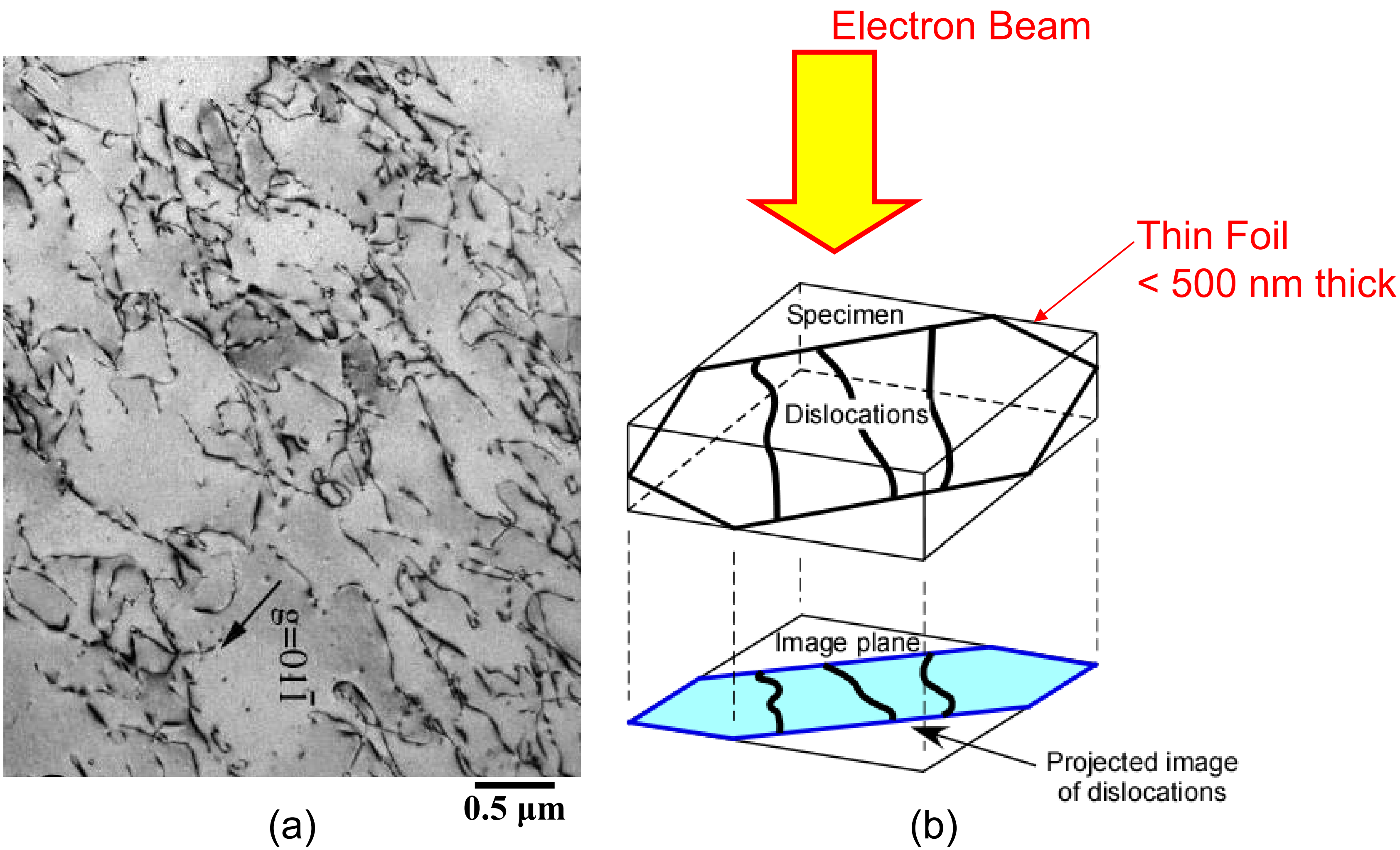
Dislocation Characteristic	Type of Dislocation		
	Edge	Screw	
Slip direction	// to *b*	// to *b*	
Relation between dislocation line and *b*	$\perp$	//	
Direction of line movement relative to *b*	//	$\perp$	
Process by which dislocations can leave slip plane	Climb	Cross-slip	

Transmission Electron Microscope (TEM)

FEI Technai F20
Super-twin

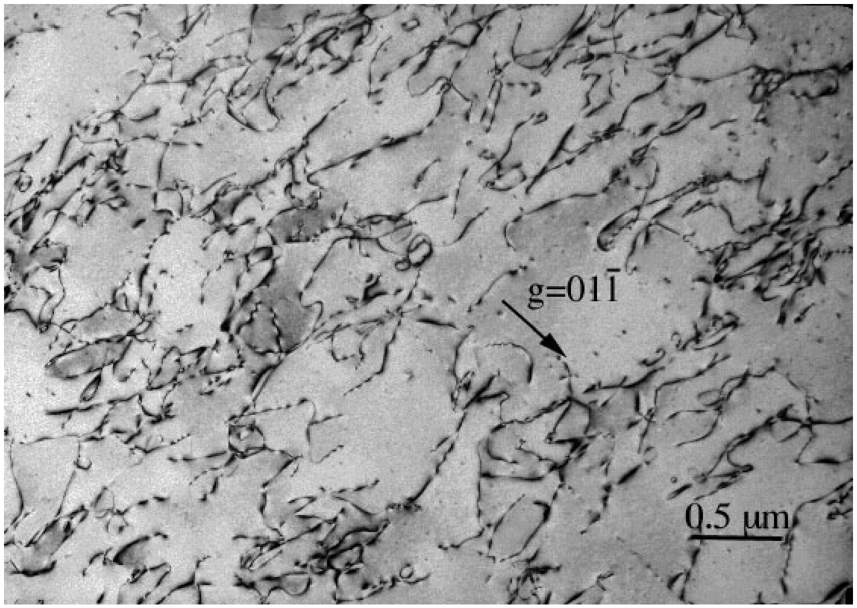


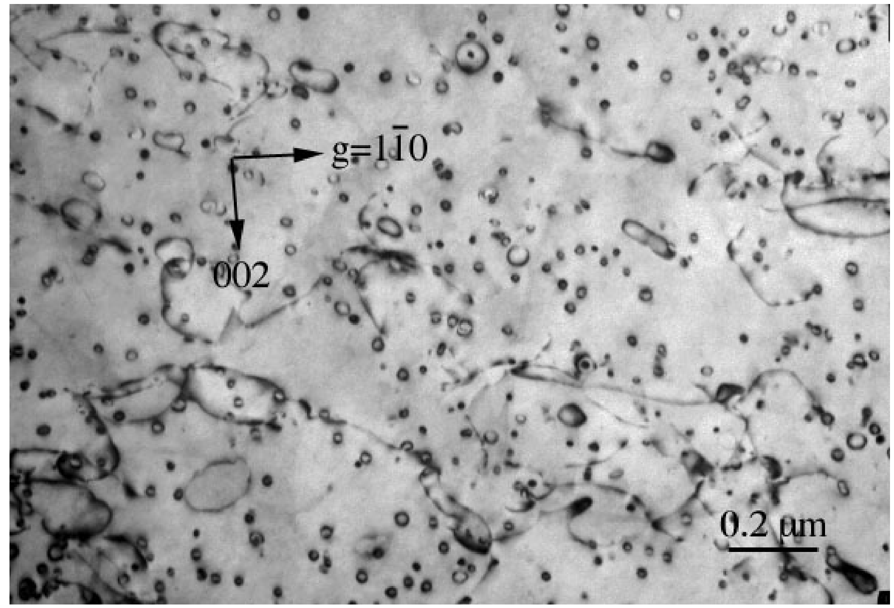
Used by materials scientists to characterize microstructures and deformation mechanisms.



(a) Transmission electron microscope image of dislocations (dark lines) in a deformed single-crystal of NiAl and (b) relationship between image and position of dislocations in thin-foil specimen. The schematic depicts three dislocations confined to a single crystallographic plane in the specimen. [Part (b) adapted from From Allen and Thomas, The Structure of Materials, (John Wiley & Sons, 1999).]

Dislocations in Crystals





[Weaver, 1995]

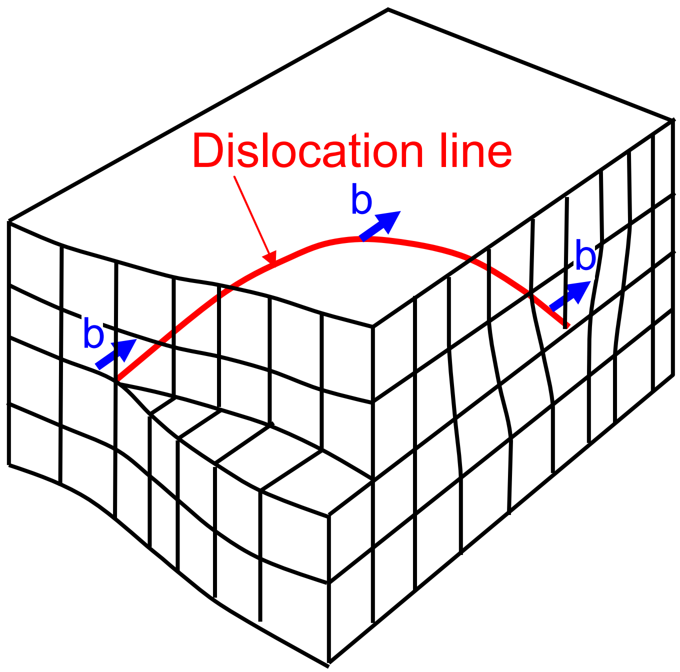
Most dislocations are curved.
Since Burgers vectors don't change, this means we need to define another type of dislocation.

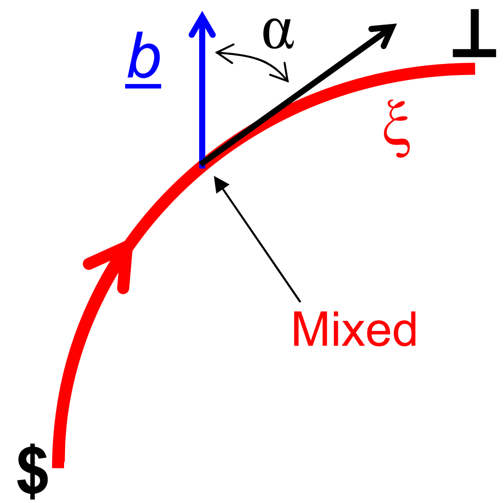
Characteristics of dislocations

Dislocation Characteristic	Type of Dislocation		
	Edge	Screw	**Mixed**
Slip direction	// to *b*	// to *b*	// to *b*
Relation between dislocation line and *b*	⊥	//	Not // or ⊥
Direction of line movement relative to *b*	//	⊥	// and ⊥
Process by which dislocations can leave slip plane	Climb	Cross-slip	Climb

The Burgers vectors for given dislocations never change!

Mixed Dislocations





The Burgers vector is oriented at some angle with respect to the dislocation line

$0° \leq \alpha \leq 90°$

Dislocations in Crystals

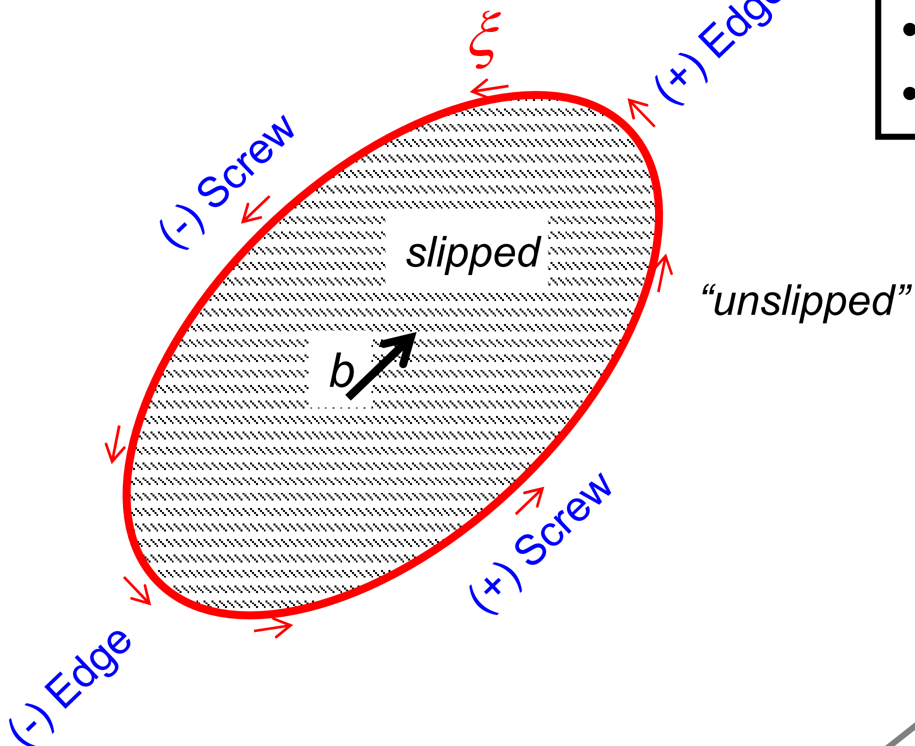
Dislocations can terminate at free surfaces, or at grain or phase boundaries; but <u>never</u> within the crystal.

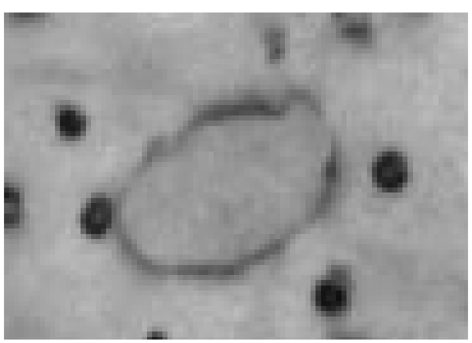
Dislocations must form closed loops or networks with branches that terminate at a surface.

The junction point within a network is called a node.

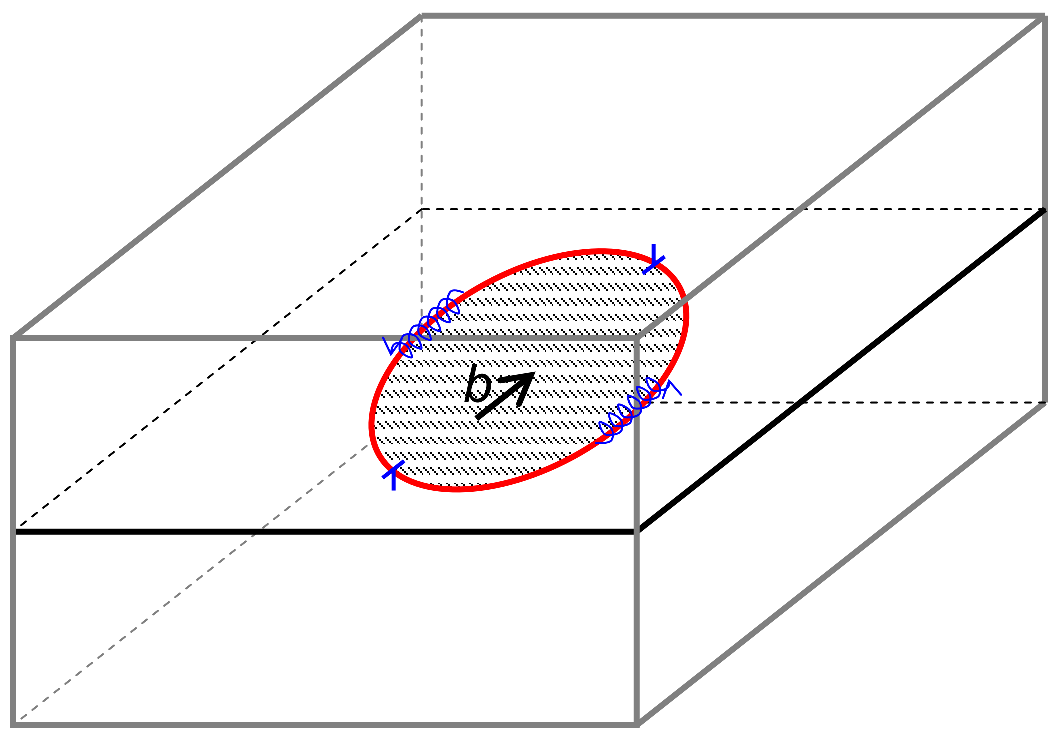
Dislocations will either:

- ►Form closed loops
- Form nodes/networks
- Emerge at the surface of a crystal.

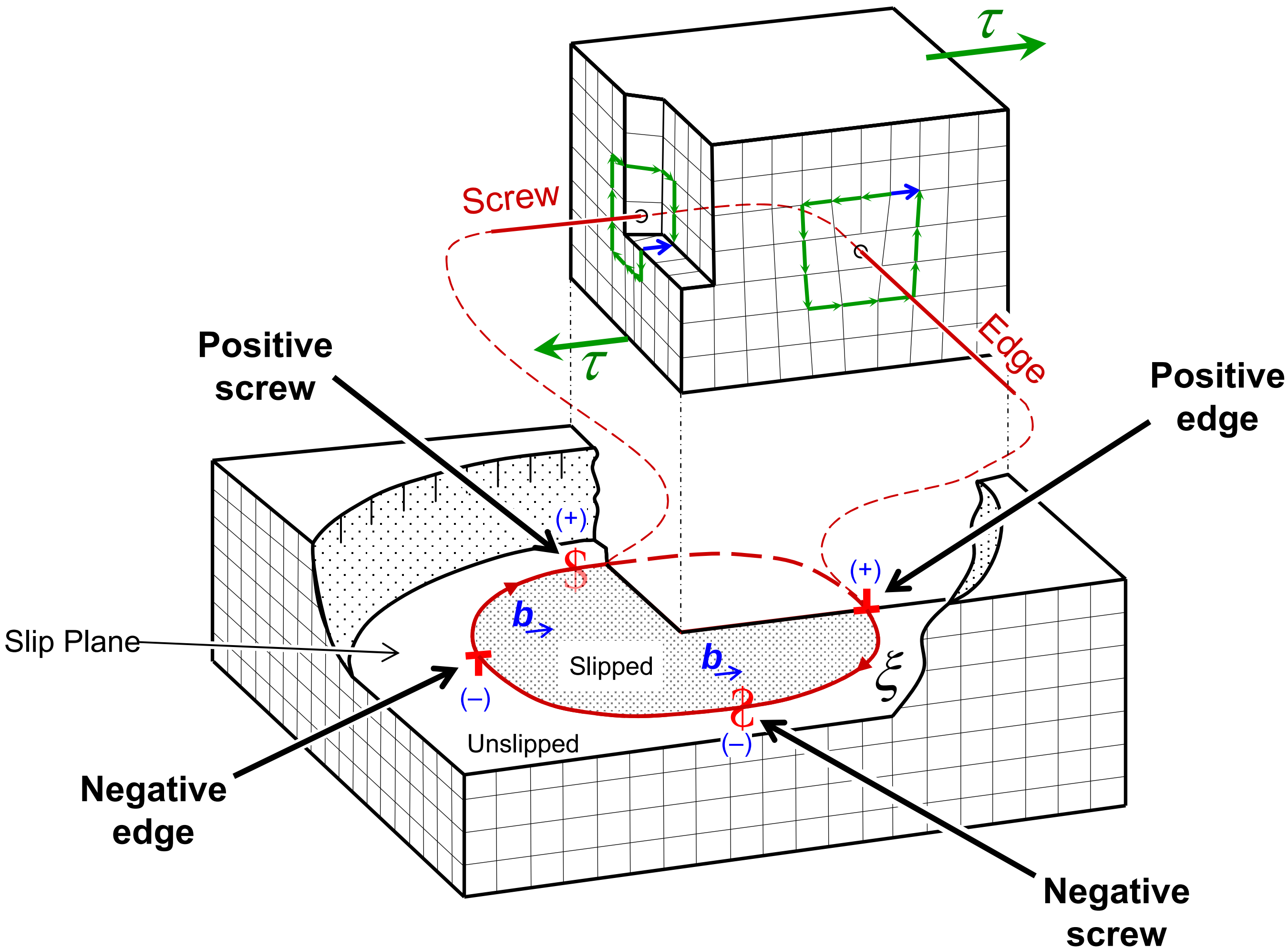




[Weaver, 1995]



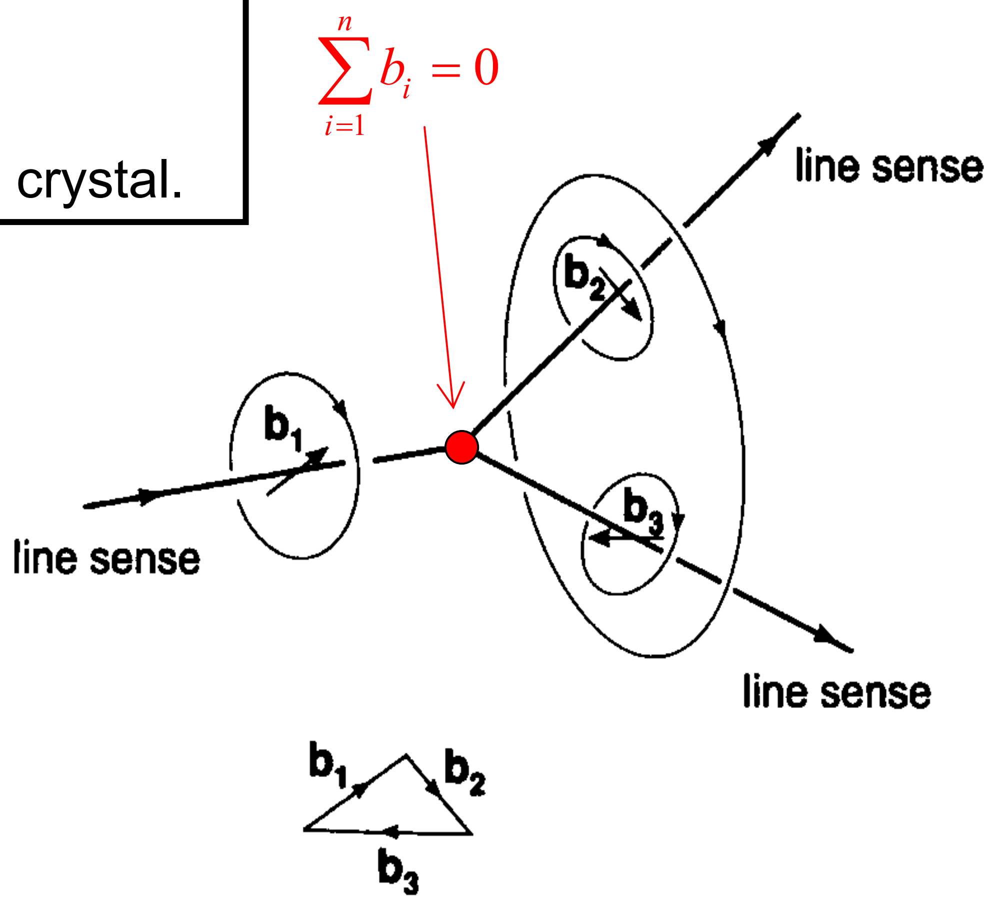
Geometry of a closed dislocation loop



This figure was adapted from H.W. Hayden, W.G. Moffatt, and J.W. Wulff, The Structure and Properties of Materials, Vol. III, (Wiley, New York 1965) p. 65.

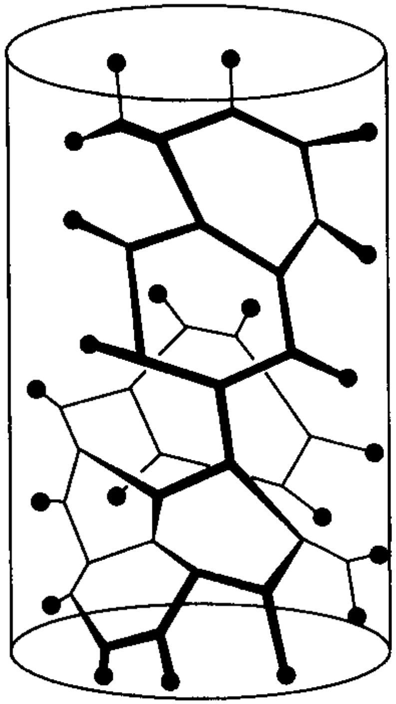
Dislocations will either:

- Form closed loops
- ►Form nodes/networks
- Emerge at the surface of a crystal.

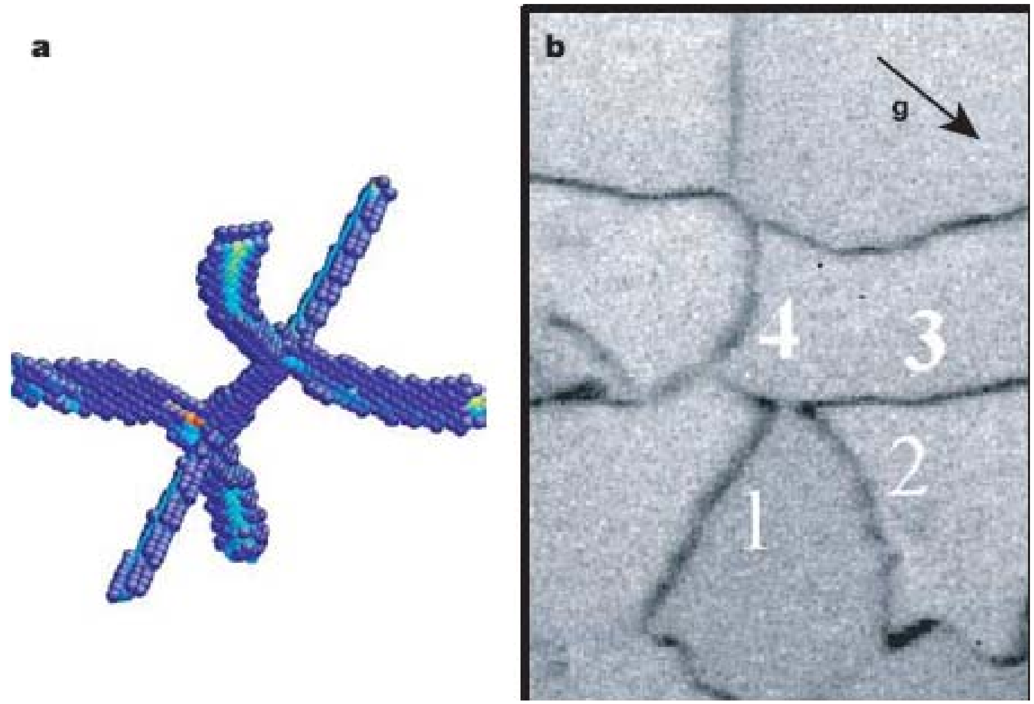


Three dislocations forming a node. From D. Hull and D.J. Bacon, Introduction to Dislocations, 4th Ed., (Butterworth-Heinemann, Oxford, 2001) p. 19.

Nodes and Dislocation Networks



Schematic of a Frank net
in a well-annealed crystal

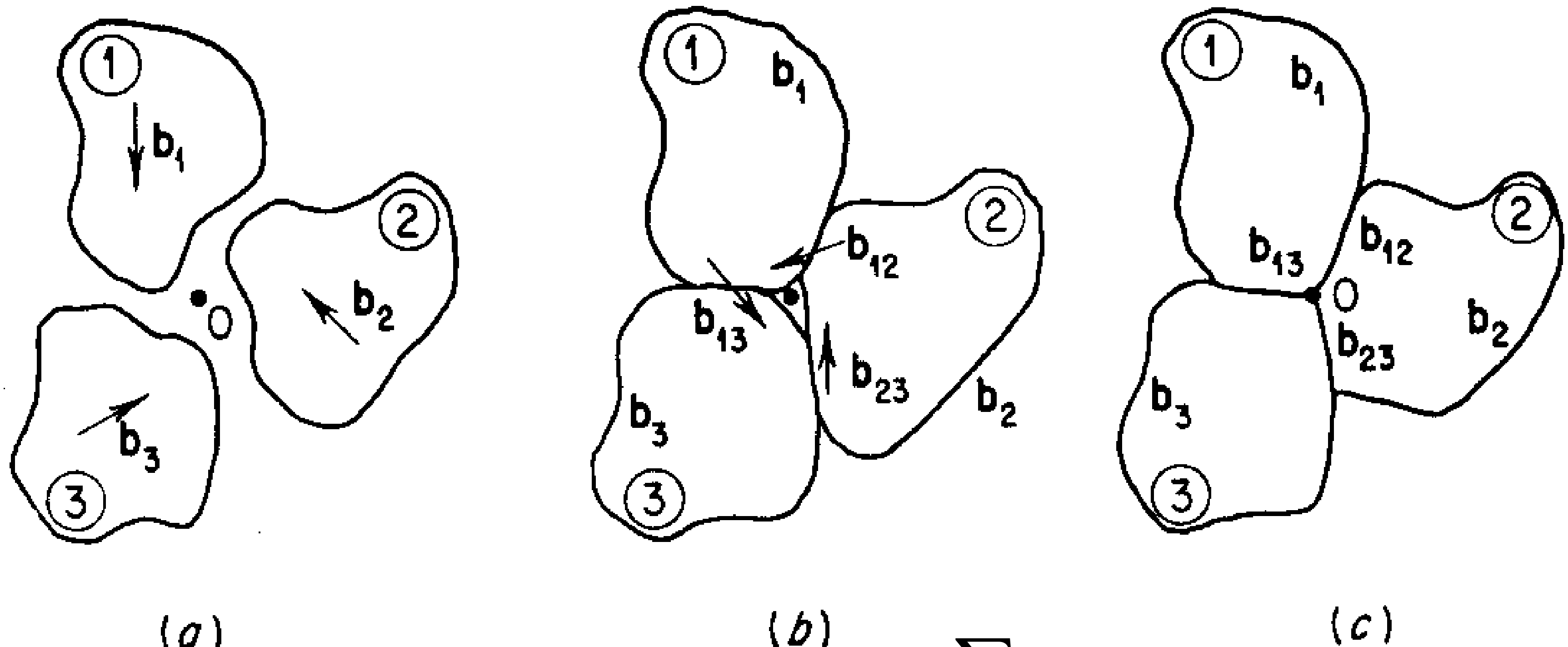


Atomic simulation and TEM image of a
symmetric 4-node in b.c.c. molybdenum

From D. Hull and D.J. Bacon, Introduction to Dislocations, 4th Ed., (Butterworth-Heinemann, Oxford, 2001) p. 20.

V.V. Bulatov, L.L. Hsiung, M. Tang, A. Arsenlis, M.C. Bartelt, W. Cai, J.N. Florando, M. Hiratani, M. Rhee, G. Hommes, T.G. Pierce and T.D. de la Rubia; “Dislocation multi-junctions and strain hardening”; *Nature*, v. 440 (2006) p. 1174.

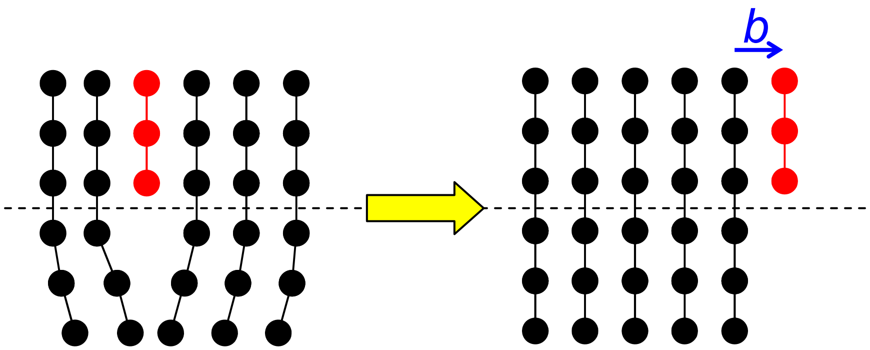
Intersection of Dislocation Loops



$$\sum_i b_i = 0$$

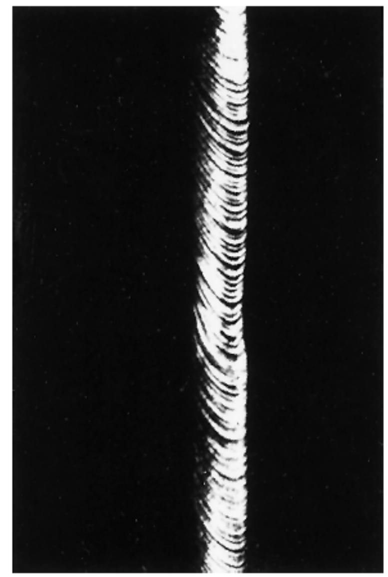
Fig. 2.8. Joining of three dislocation loops to form a node. [Figure adapted from J.J. Gilman, "Nature of Dislocations," in Mechanical Behavior of Materials At Elevated Temperatures, edited by J.E. Dorn, McGraw-Hill, New York (1961), p. 25].

Lot's of this...



After complete motion through the crystal

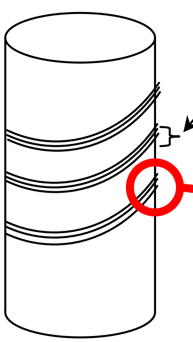
<u>Dislocations will either:</u>
- Form closed loops
- Form nodes/networks
- ▶Emerge at the surface of a crystal.

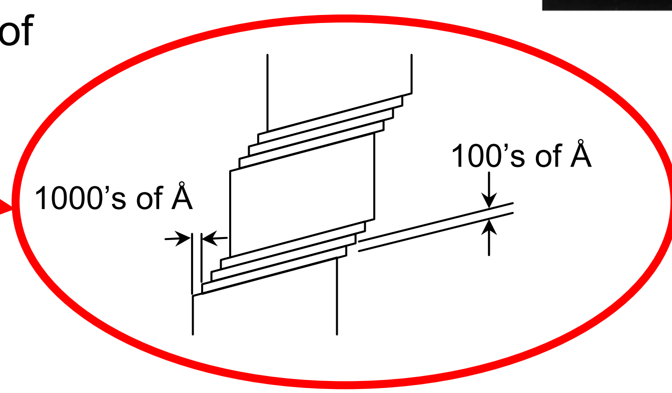


[Callister, p. 183]

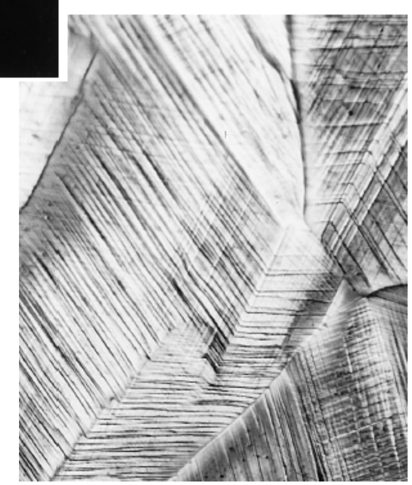
Leads to...

<u>Slip bands:</u>
Composed of several slip lines/traces





This...



[Callister, p. 186]