Welcome to
CHE 384T: Computational Methods in Materials Science

Defects in crystals

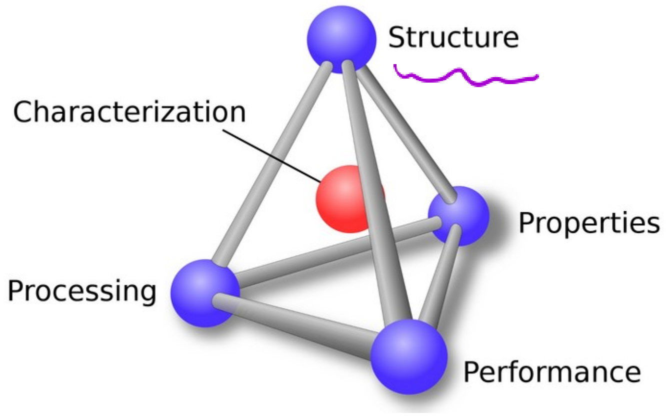
LeSar App. B1-B5

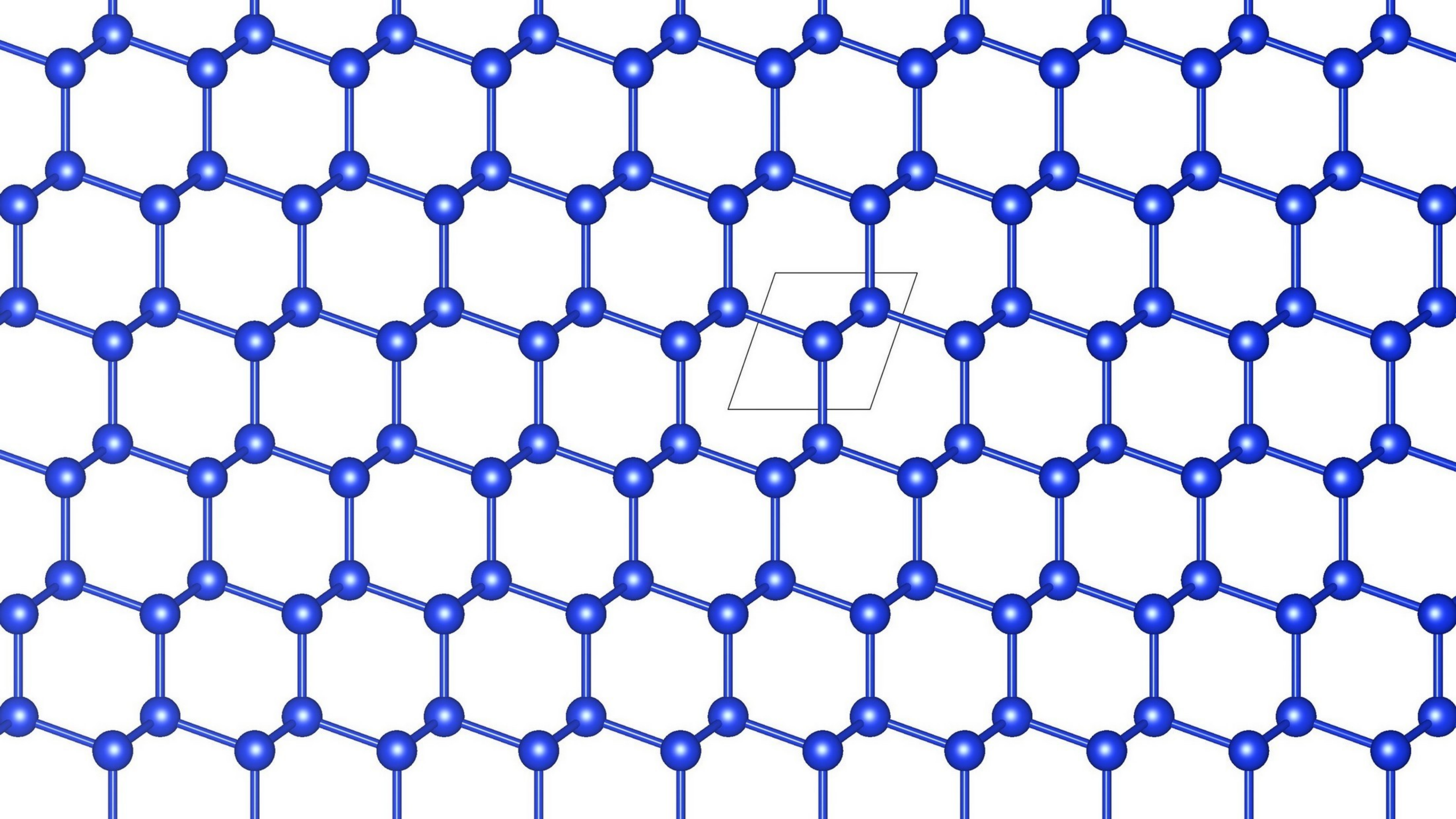
The University of Texas at Austin
McKetta Department
of Chemical Engineering
Cockrell School of Engineering

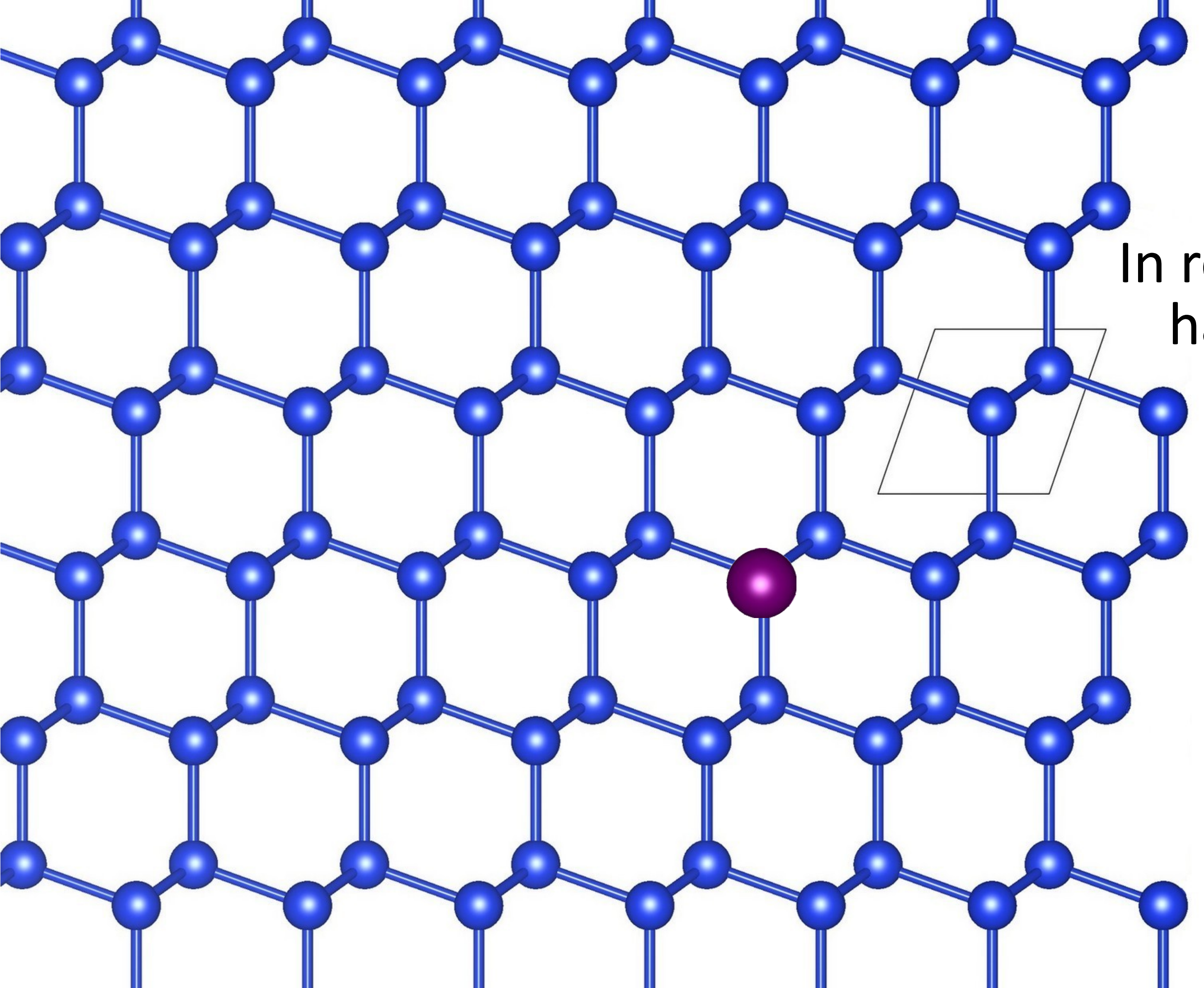
Lecture Outline

Crystal structure
- Unit cell
- Bravais Lattices
- Example Crystal structures from the cubic space group

Brief on Crystallographic notation



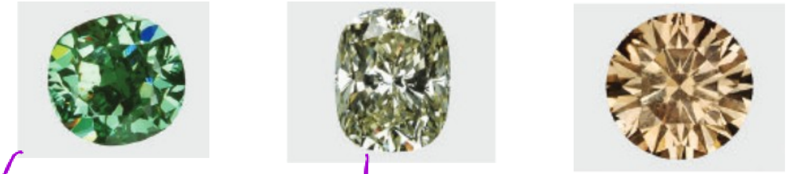




In reality, we often don't have perfect crystals

Defects can alter the properties of the host material

Optical Properties- colored diamonds



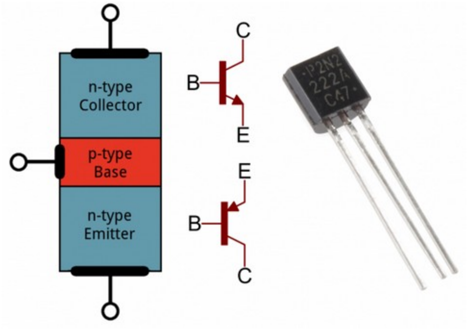
J.E. Shigley & C.M Breeding. Gems & Gemology, Summer 2013, Vol. 49, No. 2

H impurities

B

vacancy clusters

Electrical Properties



https://learn.sparkfun.com/tutorials/transistors/all

Mechanical Properties

S.E. Merzlikin et al. Practical Metallography. 48, 365-375 (2011)

H diffuses → embrittlement

Types of Defects

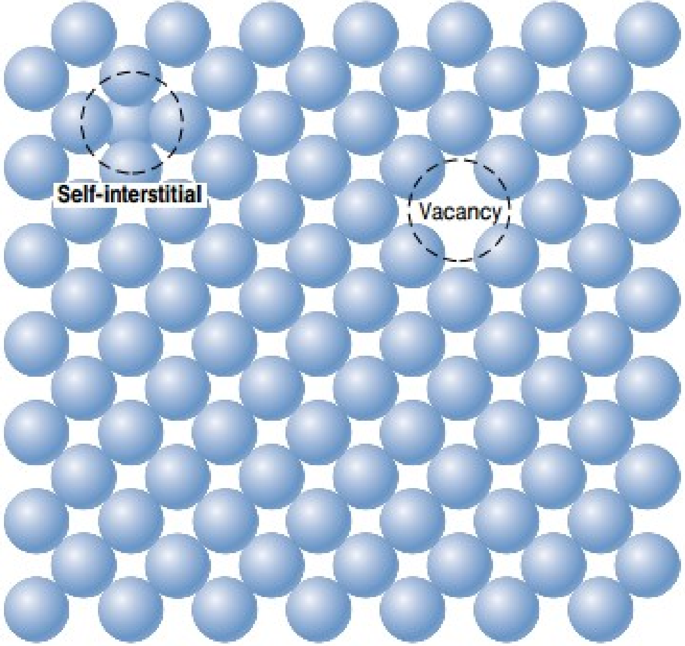
0D Point Defects: Impurities, Vacancies, Interstitials

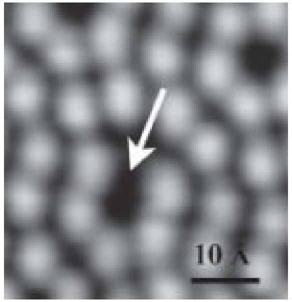
1D Line Defects: Edge and Screw Dislocations

2D Interfacial Defects: Grain boundaries

Point defects in crystals (monatomic)

Figure 4.1 Two-dimensional representations of a vacancy and a self-interstitial.
(Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 77. Copyright © 1964 by John Wiley & Sons, New York, NY. Reprinted by permission of John Wiley & Sons, Inc.)





Scanning probe micrograph that shows a vacancy on a (111)-type surface plane for silicon.

native point
points

Point defects in crystals (monatomic)

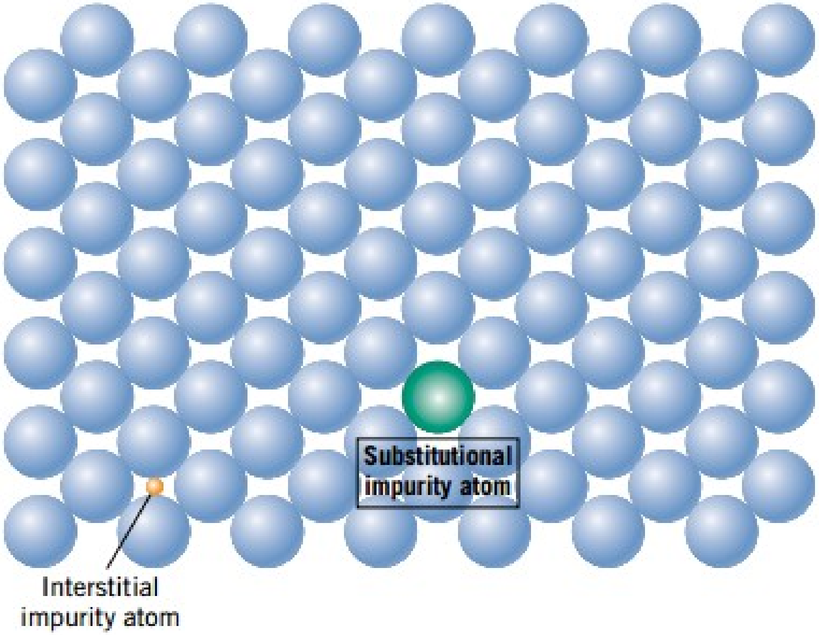
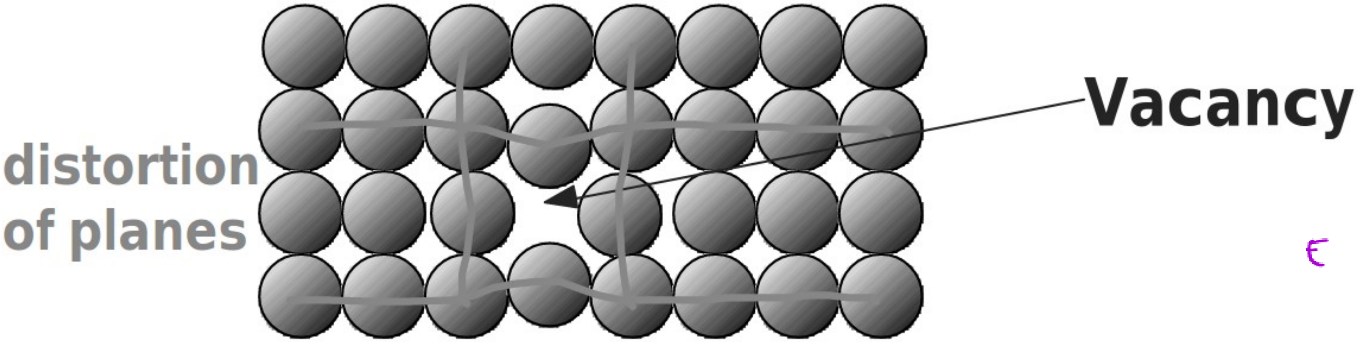
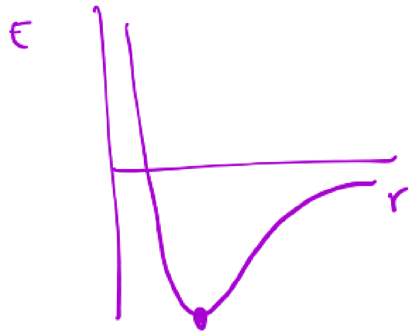


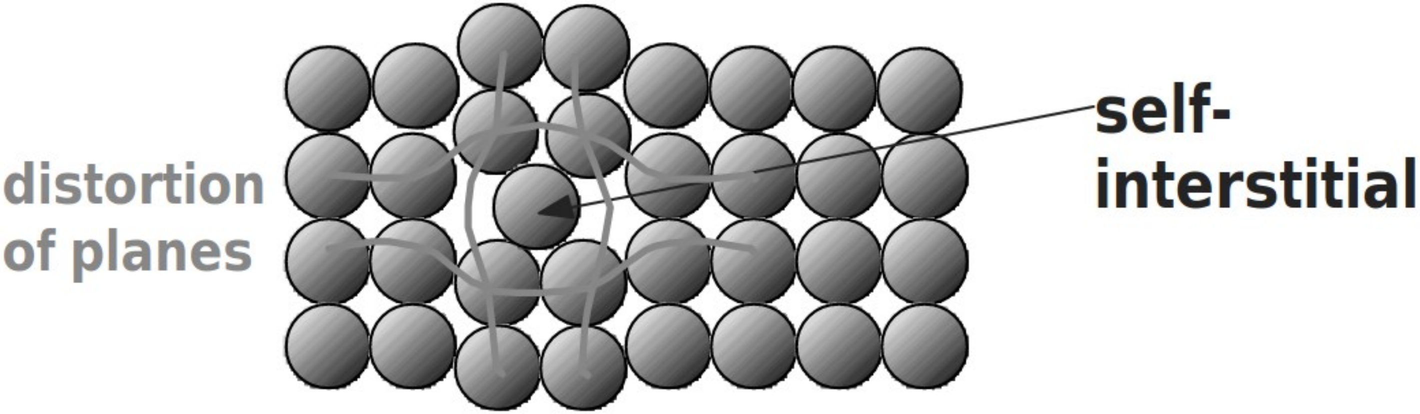
Figure 4.2 Two-dimensional schematic representations of substitutional and interstitial impurity atoms. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 77. Copyright © 1964 by John Wiley & Sons, New York, NY. Reprinted by permission of John Wiley & Sons, Inc.)

extrinsic point defects

Lattice Strain from point defects

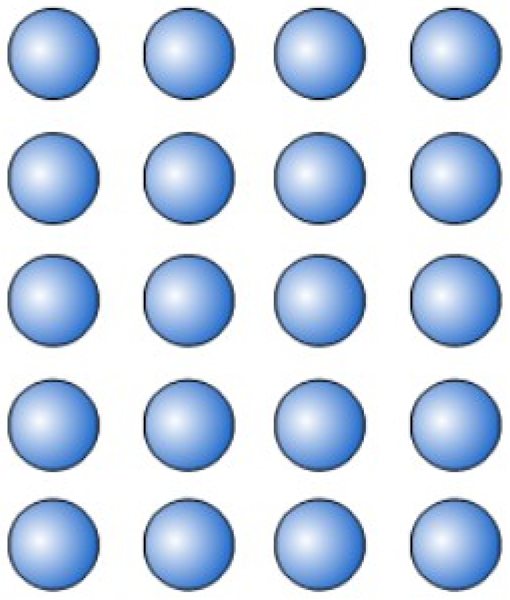




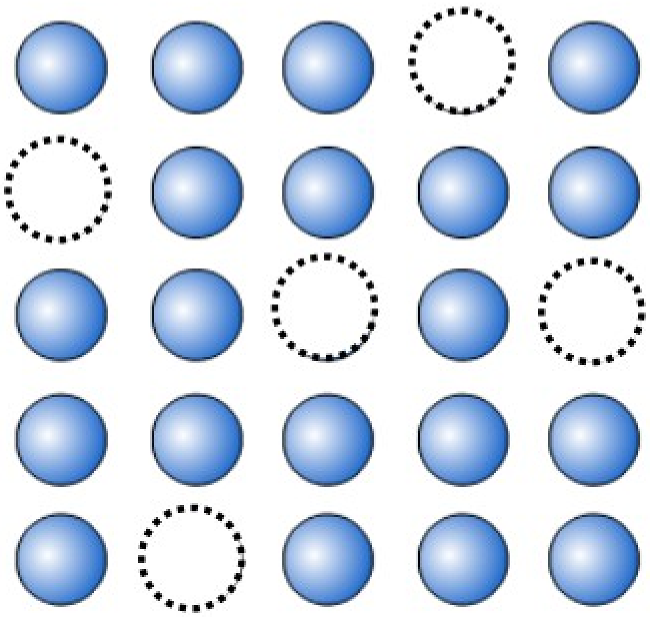


Equilibrium concentration of (point) defects

Thermodynamically, there will be some finite concentration of defects



OR



Equilibrium concentration of (point) defects

defects

lattice sites

$$\frac{n}{N} = \exp\left(-\frac{\Delta E_D}{k_B T}\right)$$

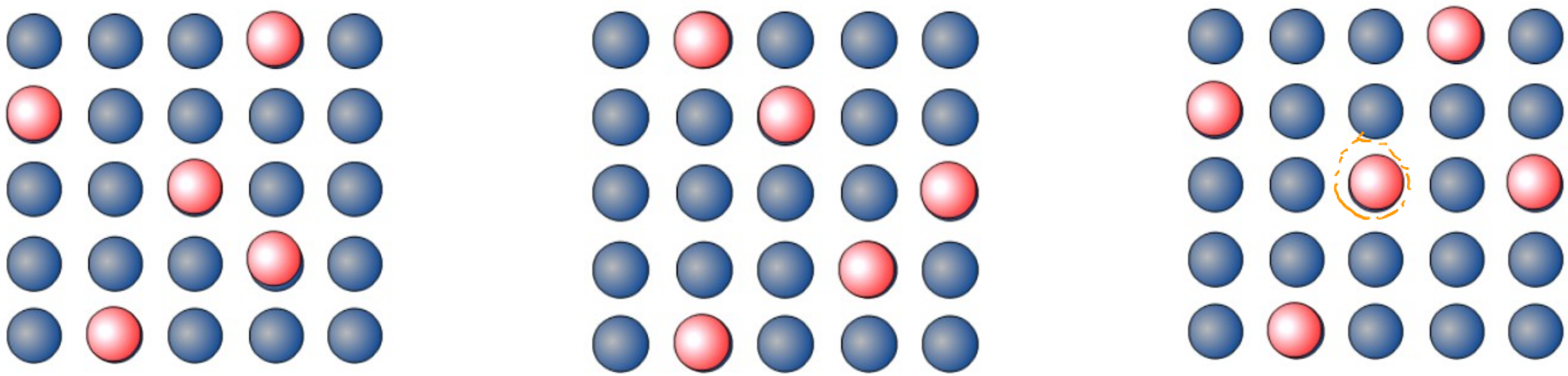
formation energy of defect

@ room temp

~ 25 meV

Equilibrium concentration of (point) defects: Microstates

Configurational Entropy: How many microstates are there for a given macrostate?



$$\Delta G = \Delta H - T\Delta S$$

configurational entropy

$$S = k_B \ln W$$

macrostate: 25 lattice sites, 5 vacancies

$$W = \frac{N!}{(N-n)!\,n!}$$

microstates: # ?

N = # lattice sites

n = # defect sites

Equilibrium concentration of (point) defects: Derivation

$$\Delta G = \underbrace{\Delta H}_{n\Delta E_D} - T\Delta S_{config}$$

$$= n\Delta E_D - Tk_B \ln W$$

$$= n\Delta E_D - k_B T \ln\left[\frac{N!}{(N-n)!\,n!}\right]$$

Stirling's approximation

$$\ln N! \approx N\ln N - N$$

@ Equilibrium

$$\Delta G = 0$$

$\Delta G > 0$ req. energy input

$\Delta G < 0$ spontaneous

$$\frac{\partial \Delta G}{\partial n} = 0$$

$$\frac{n}{N} = \exp\left(-\frac{\Delta E_D}{k_B T}\right)$$

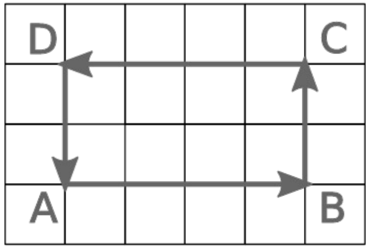
$$n \sim N \exp\left(-\frac{\Delta E_D}{k_B T}\right)$$

$T \to \infty$ $n \to N$

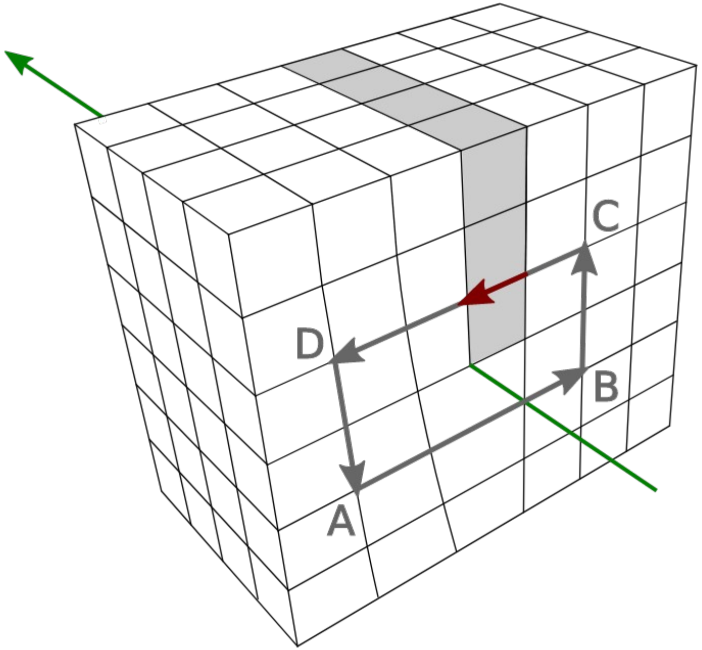
$T \to 0$ $n \to 0$

Equilibrium concentration of (point) defects: Derivation

Edge Dislocation



Burgers Vector $\vec{b}$
Dislocation Line Vector $\vec{L}$



$\vec{b}$

$\vec{L}$

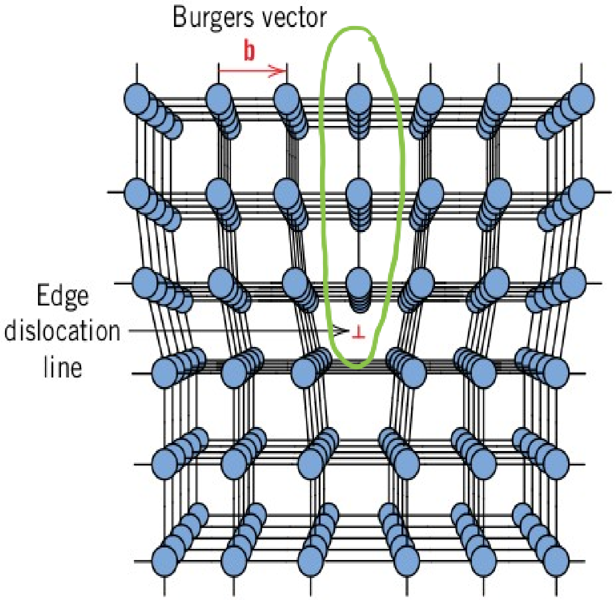
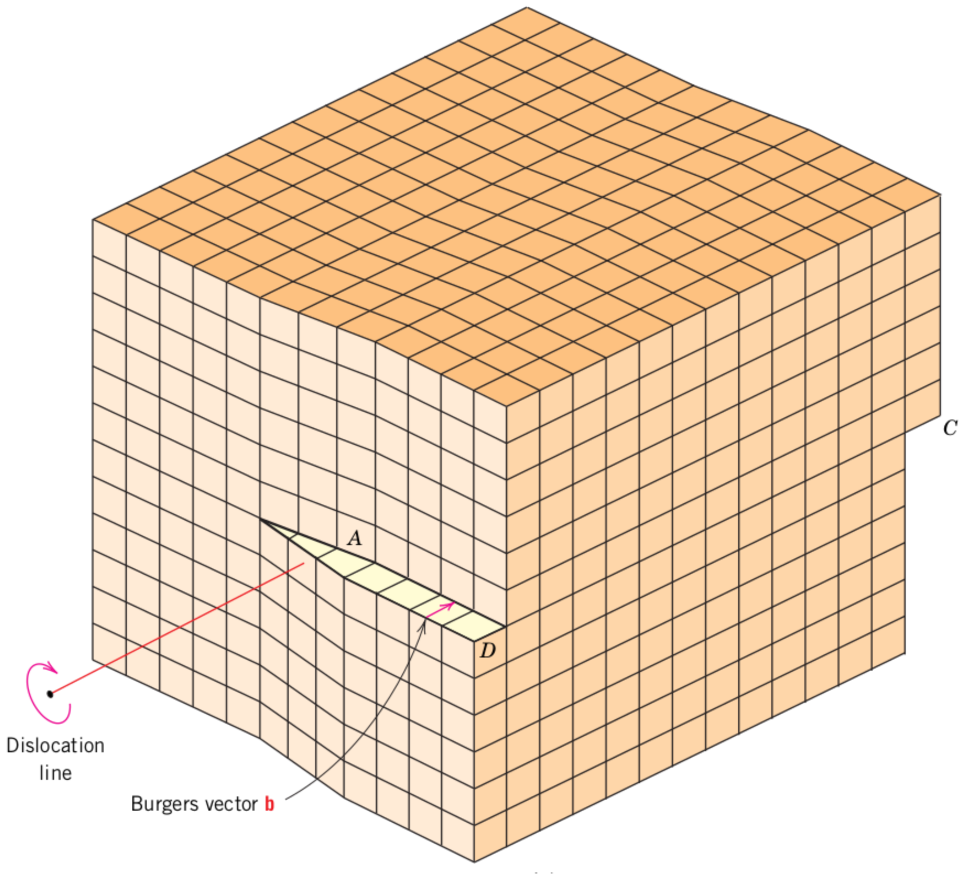


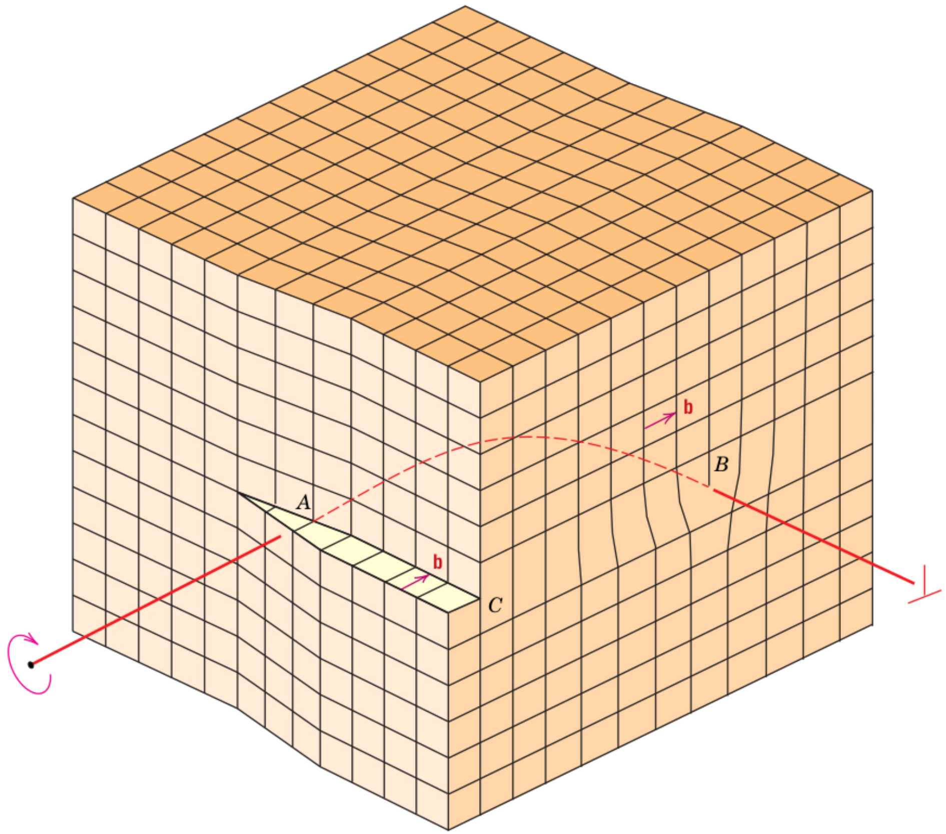
Figure 4.
edge dislc
shown in
(Adapted f
Science, M
NY, 1976,]

Screw Dislocation

Figure 4.5 (*a*) A screw dislocation within a crystal. (*b*) The screw dislocation in (*a*) as viewed from above. The dislocation line extends along line *AB*. Atom positions above the slip plane are designated by open circles, those below by solid circles.
[Figure (*b*) from W. T. Read, Jr., *Dislocations in Crystals,* McGraw-Hill Book Company, New York, NY, 1953.]



Mixed Dislocations



Plastic deformation through motion of dislocations

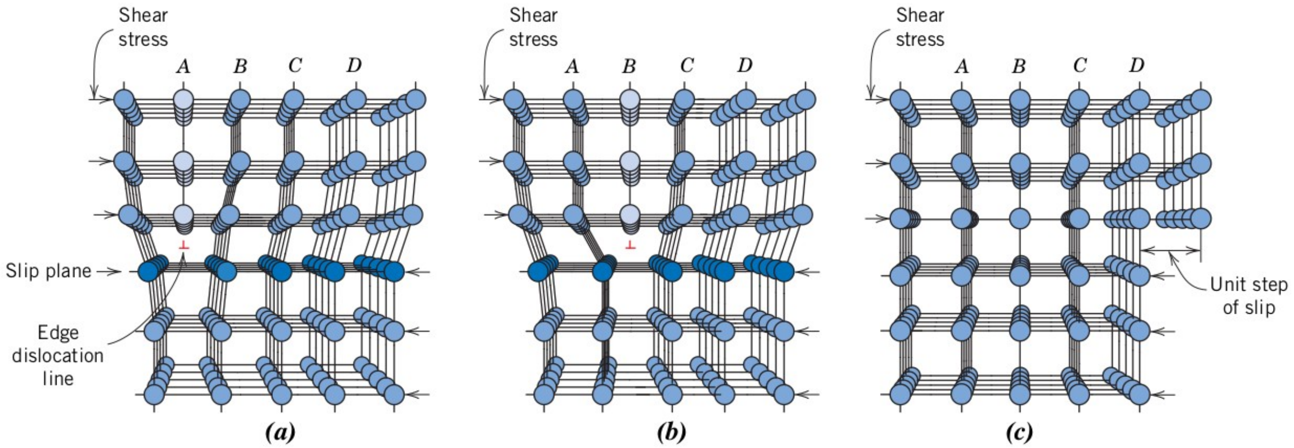


Figure 7.1 Atomic rearrangements that accompany the motion of an edge dislocation as it moves in response to an applied shear stress. (*a*) The extra half-plane of atoms is labeled *A*. (*b*) The dislocation moves one atomic distance to the right as *A* links up to the lower portion of plane *B*; in the process, the upper portion of *B* becomes the extra half-plane. (*c*) A step forms on the surface of the crystal as the extra half-plane exits.
(Adapted from A. G. Guy, *Essentials of Materials Science,* McGraw-Hill Book Company, New York, 1976, p. 153.)

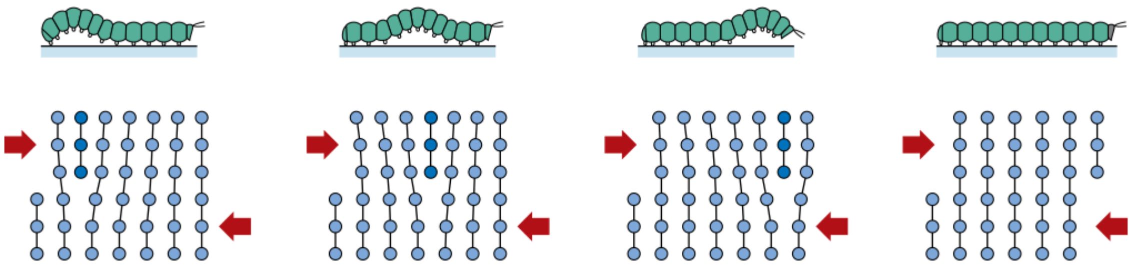
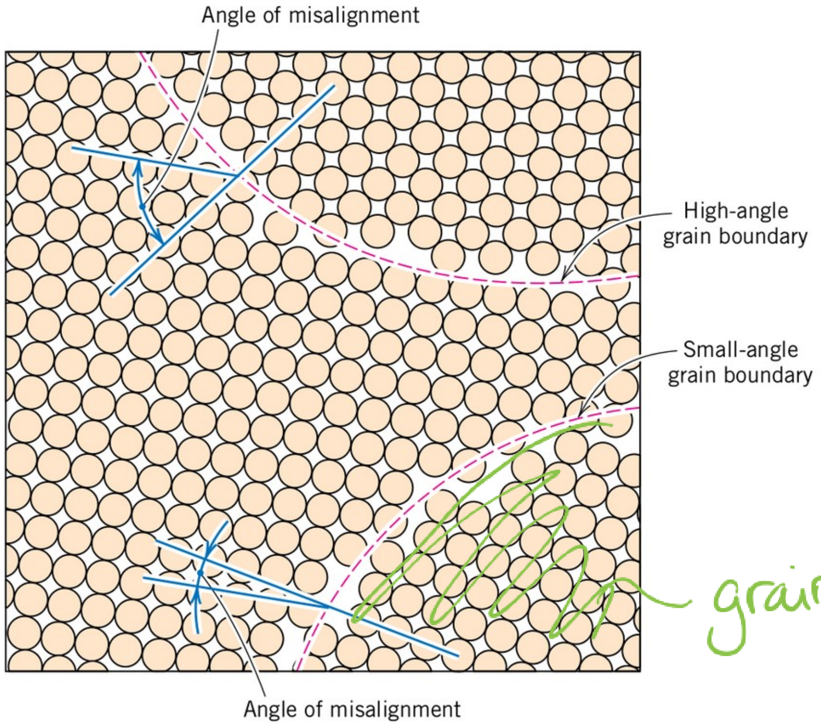


Figure 7.3 The analogy between caterpillar and dislocation motion.

Grain Boundaries



grains

Figure 4.8 Schematic diagram showing small- and high-angle grain boundaries and the adjacent atom positions.

polycrystalline

Grain Boundaries

S.E. Merzlikin et al. Practical Metallography. 48, 365-375 (2011)

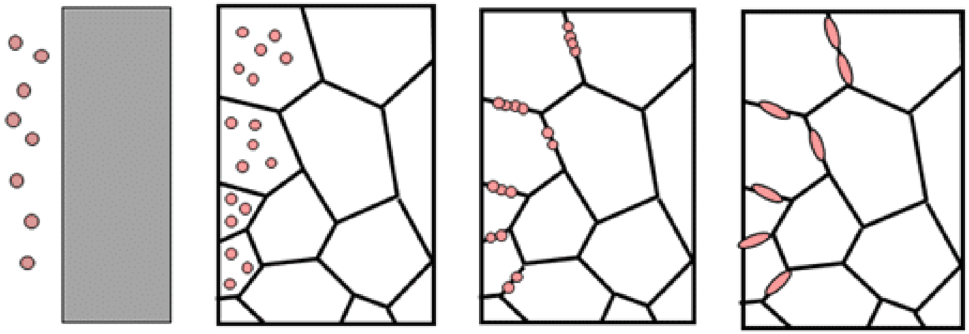


Image from Industrial Metallurgists, LLC

Bubble Raft Videos

From The Royal Institution archives

Used to understand defects in metals using a 2D HCP model

Narrated by Sir William Lawrence Bragg