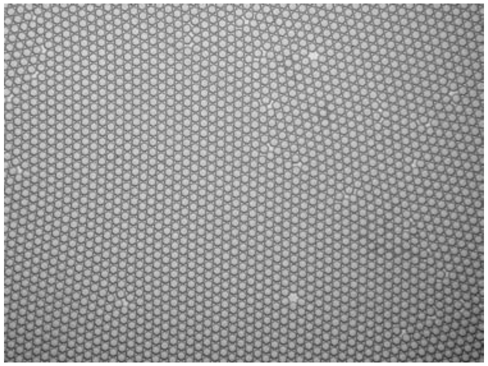
3.40J / 22.71J
Modern Physical Metallurgy

KJ Van Vliet and KC Russell

Lecture 4: 1D Crystalline Defects

February 19, 2004



Bragg-Nye Bubble Raft Model

Defects control physical and functional properties of metals

Defects control all properties of metals
- Mechanical deformation
- Electrical and thermal conductivity
- Magnetic hysteresis
- Environmental resistance (temperature, chemicals)

Since 1930s, we have known that single crystals are much weaker than predicted, so defects like dislocations were hypothesized to exist.

Not until 1950s that such defects observed experimentally with transmission electron microscopy (TEM).

Fundamental study of defects in

1D: vacancies, interstitials

2D: dislocations, twin boundaries

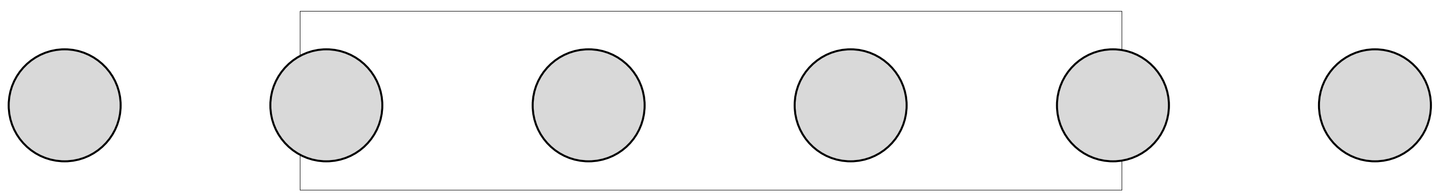
3D: grain boundaries

has greatly enhanced our ability to design for and against defect-mediated processes.

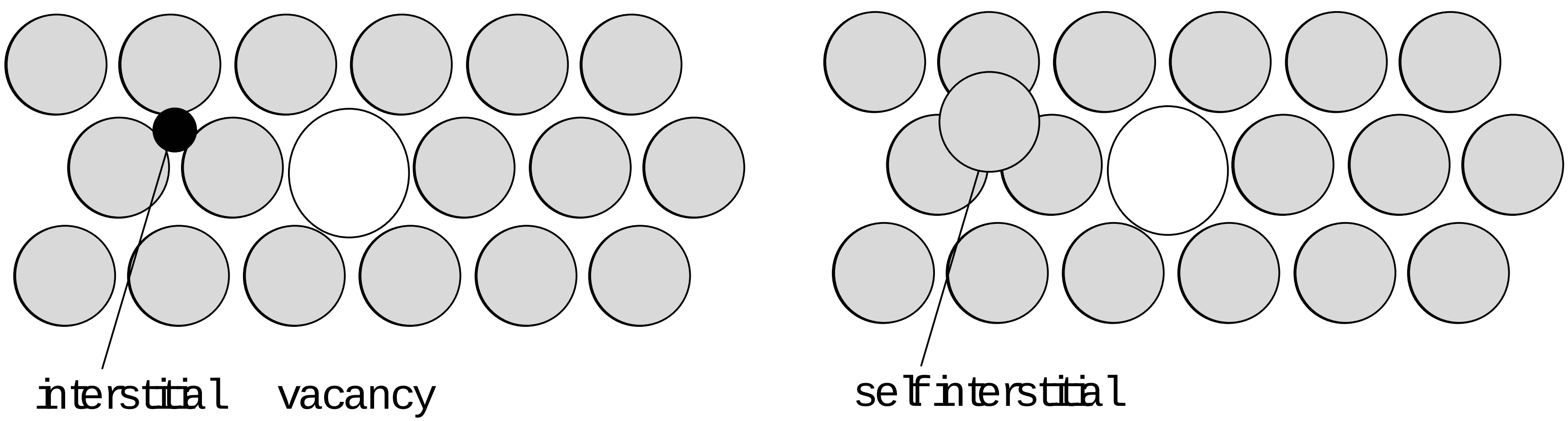
1D Defects: Vacancies and Interstitials

Two kinds of deformation

ELASTIC: reversible, bond stretching



PLASTIC: irreversible/permanent, bond breaking OR bond making



1D Defects: Vacancies and Interstitials

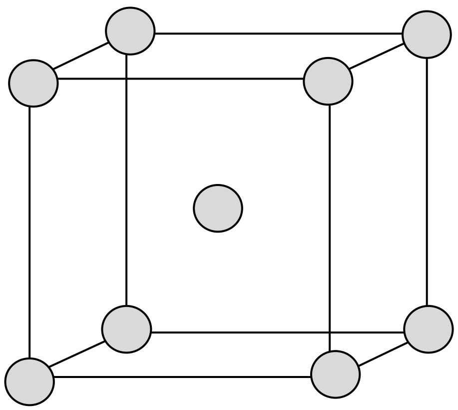
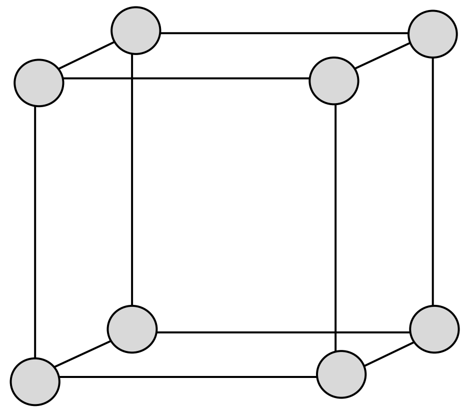
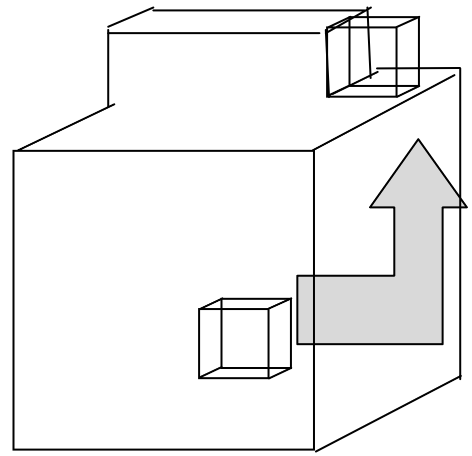
1D or Point Defects: Single missing (vacancy) or extra (interstitial) atom, with respect to crystallographic lattice sites

Energy to make these defects:

E_v ~ 1 eV/vacancy ~ 100 kJ/mol
E_i ~ 10 eV/interstitial ~ 1000 kJ/mol

Why?
Takes more energy to strain the lattice and add an atom in (I) then it does to move one to the surface (V)

1D Defects: Vacancies

Presence of a vacancy raises the energy of a crystal by a certain amount. Why?

Requires energy to remove atom from lattice and place it on surface ledge

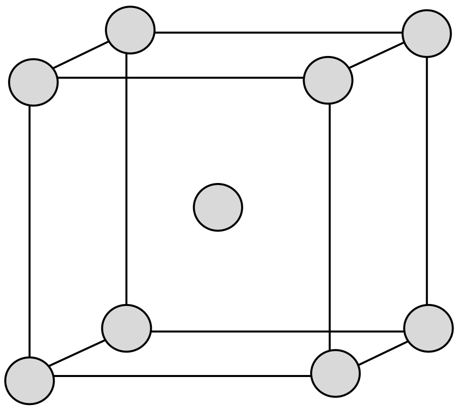
Energy = sublimation energy per atom

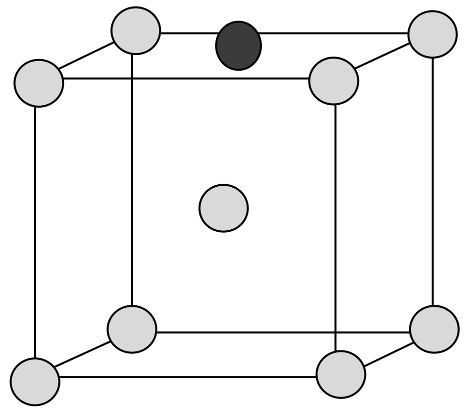
Break 6 bonds, and relocation regains 3 bonds; Sublimating same atom breaks 3 bonds.

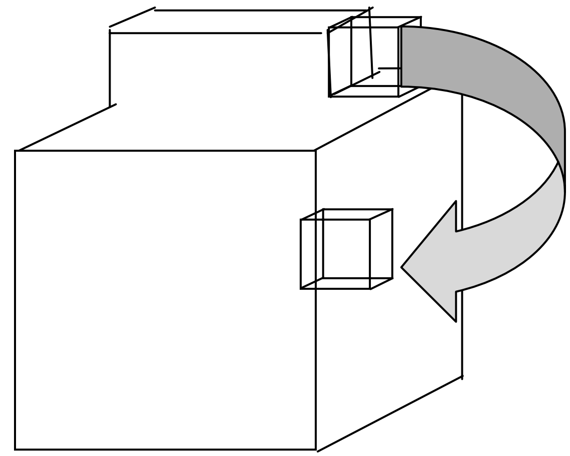
$\Delta H_{fv} = Gb^3/5 \sim 1$ eV for Cu (scales with G)

Some relaxation of atoms around the vacancy (slight contraction) in metals, but actually expansion in ionic solids due to charge interactions

1D Defects: Interstitials







Presence of an interstitial raises energy more than that of a vacancy. Why?
Requires energy to remove atom from surface ledge and jam it into the lattice → significant elastic misfit strain

Energy = sublimation energy per atom

Break 6 bonds, and relocation regains 3 bonds; Subliming same atom breaks 3 bonds.

$\Delta H_{fi} = 2Gb^3 \sim 10$ eV for Cu (scales with G)

10x greater energy to make interstitial than to make vacancy!

This argument holds for close-packed metals.

1D Defects Key Topics:

- Energy barrier to motion
- Thermal equilibrium
- Equilibrium concentration
- Lattice sites

Continued on next page.

Why do we care about 1D defects?

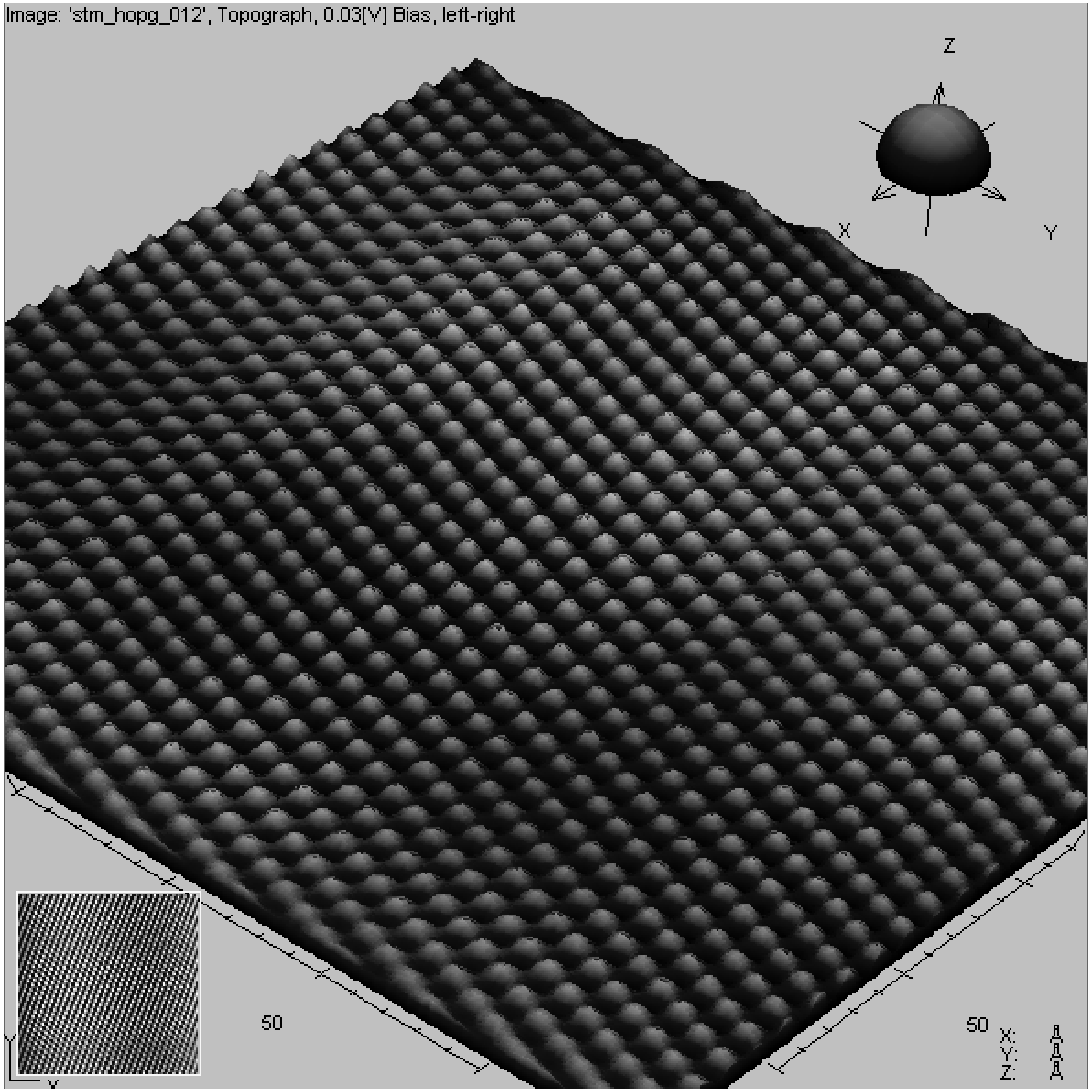
- Determining how vacancies/interstitials are created and destroyed in solids is a fundamental issue

- Determining diffusivity of vacancies is important to electronic and structural applications

- The behavior of vacancies on the surface of a material can be **directly** observed with LEEM and STM

STM Image of graphite at room temperature

No vacancies at room temperature due to increased atomic mobility



Van Vliet et al. (2004) on Molecular Imaging STM