Imperfections/Defects in Solids

- Classification of Defects in Solids:
  - ✓ **Point defects:** *Zero dimensional defects*
    - o Vacancies
    - o interstitials
    - o foreign atoms
  - ✓ **Line defects:** *One dimensional defects*
    - o dislocations
  - ✓ **Planar defects:** *Two dimensional defects*
    - o Interfaces
    - o grain boundaries
  - ✓ **Bulk or Volume defects:** *Three dimensional defects*
    - o Precipitates
    - o vacancy agglomerates
  - ✓ **Crystallinity:**
    - o single, poly, amorphous

MSE 310
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Knowlton

Imperfections/Defects in Solids

- Why would we want to study defects?
  - ✓ Defects affect primarily all properties of materials
    - o Electrical
      - All defects, especially point defects
    - o Optical
      - All defects, especially point defects
    - o Mechanical (eg., strength, toughness, hardness, etc)
      - All defects, especially dislocations
    - o Magnetic
      - All defects
    - o Kinetic (e.g., diffusion):
      - All defects, especially point defects

Imperfections/Defects in Solids

- Point defects differ from 1D (line) or 2D defects in two important respects
  - ✓ *Point defects* are difficult to observe directly.
  - ✓ Thus, *Point defects* are usually are detected and studied through their effect upon some physical property of the material.
  - ✓ They may be present in appreciable concentrations even though the material is in thermodynamic equilibrium.
    - o While *dislocations* and *interfaces* raise the **free energy** of a material, adding a certain number of *point defects* to an otherwise perfect crystal reduces its **free energy** to a minimum value.
    - o This is because of a *gain of entropy* caused by the many possible sets of places in the crystal in which the *point defects* can exist.
    - o This has to do with *Configurational* or *Statistical Entropy*, which is determined using *Statistical Thermodynamics/Mechanics*.

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Imperfections/Defects in Solids

- Question: How many vacancies are needed to minimize the *Free Energy* a crystalline material?

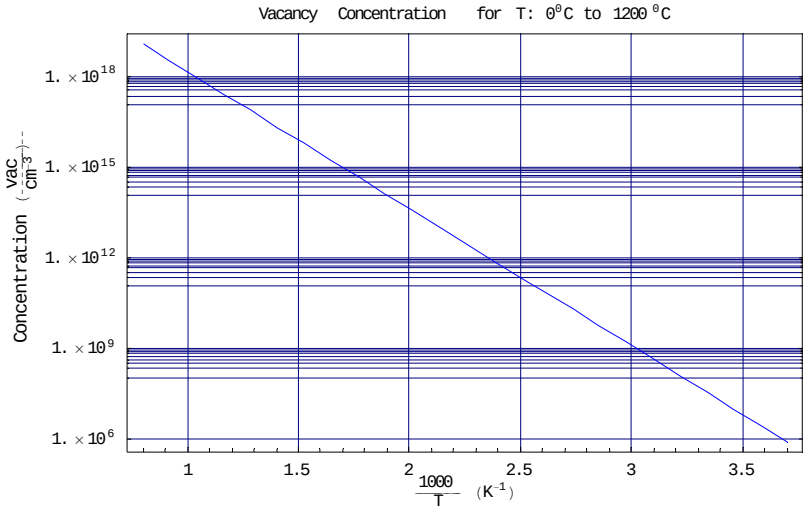
$$n_v = n_{bulk} e^{-(E_f)/kT}$$

- n_v: density of vacancies in bulk crystal
- n_{bulk}: density of atoms/lattice sites in bulk crystal
- E_f: energy of formation/activation of vacancies
- k_b: Boltzmann's constant
- T: temperature

4

Imperfections/Defects in Solids

$$n_v = n_{bulk} e^{-(E_f)/kT}$$



Imperfections/Defects in Solids

- Point defects essentially come in two flavors:
  - ✓ Native (i.e., intrinsic) point defects
    - o Intrinsic to the material
    - o Not a foreign atom or impurity
  - ✓ Extrinsic point defects
    - o Foreign atom
    - o Impurity atom
    - o Not native to the material

- Native/Intrinsic point defects:
  - ✓ Vacancies
  - ✓ Self interstitials
  - ✓ Antisite defects
  - ✓ Native complexes/pairs
    - o Frenkel defect (next slide)
    - o Schottky defect (next slide)
    - o Interstitialcy (e.g., self interstitial pairs)
    - o Multiple vacancies

Vacancies & Interstitials

❑ Native Defects - Vacancies and Interstitials

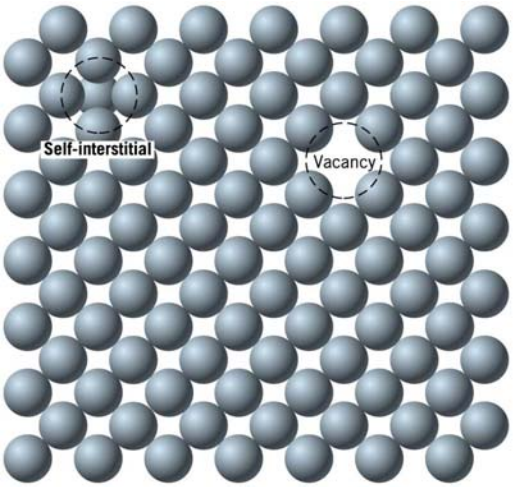


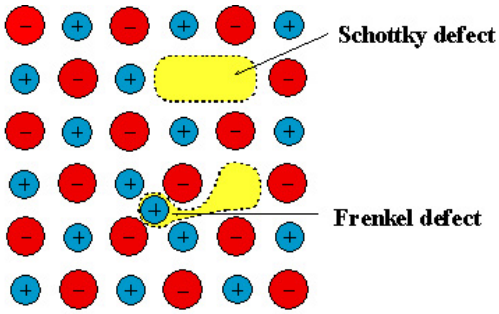
FIGURE 4.1 Two-dimensional representations of a vacancy and a self-interstitial. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 77. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley &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

Materials Science and Engineering – An Introduction, William D. Callister, Jr. 6th Ed (Wiley, 2003)

Imperfections/Defects in Solids

✓ Native complexes/pairs

- o Frenkel defect: an interstitial-vacancy pair not necessarily adjacent to one another.
- o Schottky defect: an anion (e.g., As) vacancy and cation (e.g., Ga) vacancy pair separated from one another.

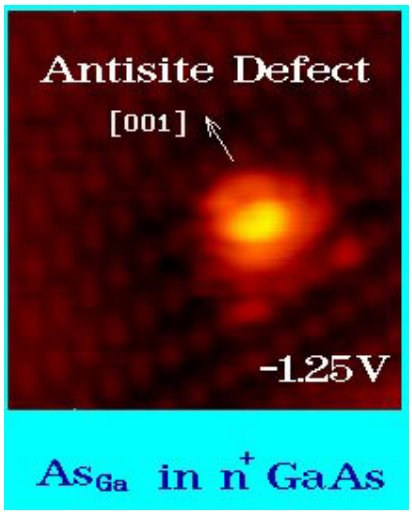


Schottky and Frenkel defects in an ionic crystal.

Kasap, Electronic Materials & Devices, 3re Ed (McGraw Hill, 2006)

Imperfections/Defects in Solids

- Example of a Native Point Defect
  - ✓ Antisite defects in GaAs



E. Weber et al., UC Berkeley & LBNL

Imperfections/Defects in Solids

- Extrinsic point defects
  - ✓ Substitutional impurity atom:
    - o Shallow acceptors
    - o Shallow donors
  - ✓ Interstitial impurity atom:
    - o Interstitial diffusers: H, Fe, Cu, Ni, O, etc.
    - o "Part time" interstitials: Al, C, B, etc.
  - ✓ Extrinsic point defect complexes/pairs:
    (A & B = *foreign atom*; V = *vacancy*; I = *Self interstitial*)
    - o AV: A = O, Ge, Sn, P, As, Sb, B, Al, etc.
    - o AI: A = C, ,B, Al, Ga, O, etc.
    - o AA or AB:
      - AA: C, N, etc.
      - AB: C_iAs_s, C_iP_s, C_iSb_s, Fe_iAl_s, etc.

Point Defect

- Extrinsic Defects - Substitutional and Interstitial

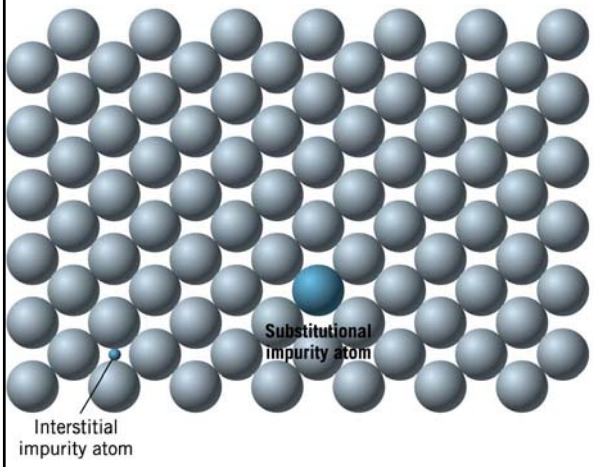


FIGURE 4.2 Two-dimensional schematic representations of substitutional and interstitial impurity atoms. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I, *Structure,* p. 77. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission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

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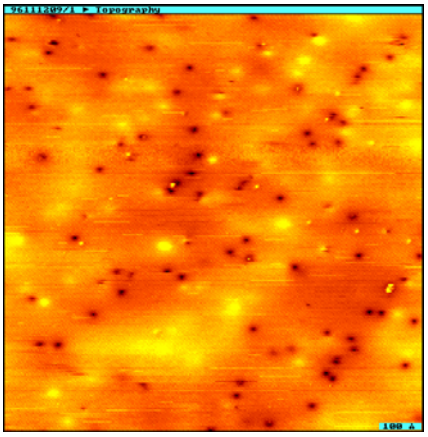
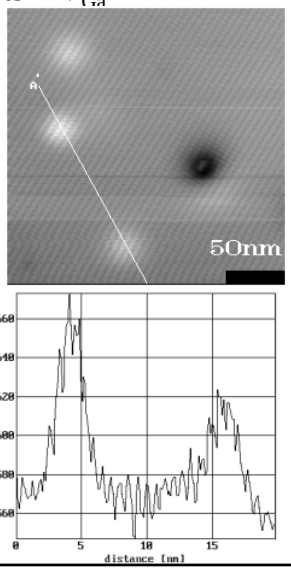
Imperfections/Defects in Solids

- Substitutional extrinsic point defects in GaAs

Light points = Si; Dark points = V_{Ga}





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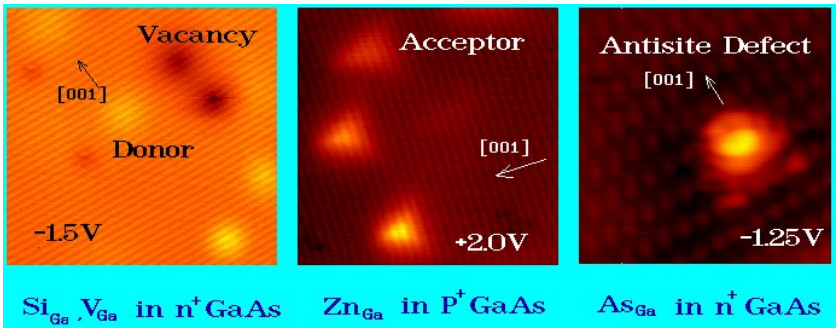
Imperfections/Defects in Solids

- Substitutional extrinsic point defects in GaAs

  Light points = donor or acceptor; Dark points = V_{Ga}



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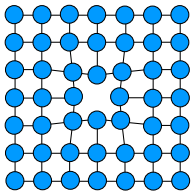
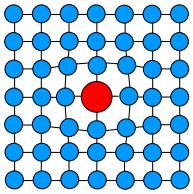
Imperfections/Defects in Solids

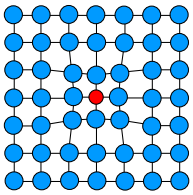
- Point defects
  - ✓ Interrupt periodicity
  - ✓ Cause strain



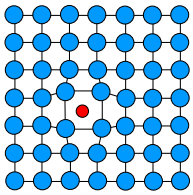
(a) A vacancy in the crystal.



(b) A substitutional impurity in the crystal. The impurity atom is larger than the host atom.



(c) A substitutional impurity in the crystal. The impurity atom is smaller than the host atom.



(d) An interstitial impurity in the crystal. It occupies an empty space between host atoms.

Fig. 1.44: Point defects in the crystal structure. The regions around the point defect become distorted; the lattice becomes strained.

Kasap, Electronic Materials & Devices, 3re Ed (McGraw Hill, 2006)