PHYSNET

MISN-0-338

LATTICE DEFECTS

Solid State Physics

Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

LATTICE DEFECTS

by

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Title: **Lattice Defects**

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Version: 2/24/2000 Evaluation: Stage B1

Length: 2 hr; 9 pages

Input Skills:

1. Vocabulary: absolute temperature, internal energy (MISN-0-157); entropy (MISN-0-160).
2. Discuss the binding mechanism and properties of an ionic solid (MISN-0-334).
3. Draw the unit cell for the simple cubic and face centered cubic lattice (MISN-0-335).

Output Skills (Knowledge):

K1. Vocabulary: native point defect,vacancy, interstitial, Schottky defect, Frenkel defect, edge dislocation, screw dislocation, energy of formation, thermodynamic probability.

K2. Calculate the maximum radius of an interstitial atom within a crystal of touching hard spheres of given radius in: (a) simple cubic structures; (b) face centered cubic structures.

K3. Derive the additional configurational entropy for the formation of vacancies in a crystal as a function of the number of lattice sites and vacancies.

K4. Derive an expression for the number of expected vacancies in a crystal in terms of the temperature and the energy of formation given the additional configurational entropy.

K5. State how an experimenter can obtain specified defects in crystal lattices.

External Resources (Required):

1. J. Blakemore, Solid State Physics, W.B. Saunders Co. (1974).

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New authors, reviewers and field testers are welcome.

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1. Introduction

So far we have been concerned with the properties, descriptions, and symmetries of perfect lattices. We will, in this unit, consider some of the types of defects that are found in crystals and learn the surprising fact that a number of defects in a crystal are necessary for it to be in thermodynamic equilibrium.

2. Comments

1. For Output Skill K4, you are given that the additional configurational entropy for the formation of n vacancies in a crystal of N atoms is

$$\Delta S = k\ell n \left[\frac{N!}{(N-n)!N!}\right]$$

where k is Boltzmann's constant. You are to show that the number of vacancies expected in the crystal in thermodynamic equilibrium is given by

$$n \simeq N e^{-E/kT} \,,$$

where E and T are respectively the energy of formation of a vacancy and the absolute temperature.

2. For Output Skill K3, you are given that the configurational entropy of a crystal of N lattice sites is

$$S = k\ell n\, W \,,$$

where W is the thermodynamic probability for the crystal, i.e. it is the number of microstates corresponding to a given macrostate. You are to show that the additional configurational entropy for the formation of n vacancies is

$$\Delta S = k\ell n \left[\frac{N!}{(N-n)!N!}\right] .$$

3. Procedures

1. Adequate definitions for each of the words listed in Output Skill K1 are to be found in section 1.6 of Blakemore. Read the section, locate the items, and write out the definitions in your own words.

2. Work the following two problems:

   Calculate the maximum radius of a hard spherical atom that would fit in an interstitial position of a crystal composed of hard spheres of radius R close-packed in the

   a. simple cubic structure, and

   b. face-centered cubic structure

3. You can obtain Output Skill K4 by working through the material in Blakemore from equation (1-57) through (1-60) in section 1.6. What you may need to review are:

   a. Stirling's approximation for the logarithm of a factorial which for large !N! is:

$$\ell n\, N! \simeq N \ell n\, N - N + \frac{1}{2}\ell n\,(2\pi N)$$
$$\simeq N\ell n\, N - N \,.$$

   b. The Helmholtz free energy, F, for a system is a minimum when the system is in thermodynamic equilibrium. This implies that

$$\left.\frac{\partial F}{\partial X}\right]_{Y,Z} = \left.\frac{\partial F}{\partial Y}\right]_{Y,Z} = \left.\frac{\partial F}{\partial Z}\right]_{X,Y} = 0 \,. \qquad \text{(at equilibrium)}\,,$$

   where $F = F\,(X, Y, Z, X\prime, Y\prime, Z\prime)$. From thermodynamics, we learn that the Helmholtz function is defined as

$$F = U - TS \,,$$

   where U, T, and S are respectively the internal energy, absolute temperature, and entropy of the system. In the derivation in the text, the internal energy of the system of vacancies in the crystal is $u = nE$, where n is the number of vacancies and E is the energy of formation for one vacancy.

   One more point to keep in mind is that even though N and n are very large numbers, N is always much larger than n.

4. Estimate the number of vacancies per atom at thermal equilibrium for a crystal at $T = 300\,\mathrm{K}$ and $T = 600\,\mathrm{K}$, assuming that the energy required to form a vacancy is $1\,\mathrm{eV}$. How many atoms are there for each vacancy at the above temperatures?

5. A complete review of material for Output Skill K3 is contained in Chapter 14 of Sears' textbook, especially section 14-4. However, if you can work the following two problems, you ought to be able to justify that the configurational thermodynamic probability for n vacancies in N lattice sites is given by

$$W_{conf} = \frac{N!}{(N-n)!n!}$$

Given N boxes and n indistinguishable balls, where both N and n are large numbers but $N > n$, show that:

a. If there are no restrictions on the total number of balls in any given box then the number of ways the balls can be distributed in the boxes is

$$\frac{(N+n)!}{N!n!}.$$

b. If each box may contain either one ball or no balls then the number of ways the balls can be distributed in the boxes is

$$\frac{N!}{(N-n)!n!}$$

Acknowledgments

The author would like to thank Illinois State University for support in the construction of this lesson. Preparation of this module was supported in part by the National Science Foundation, Division of Science Education Development and Research, through Grant #SED 74-20088 to Michigan State University.