# Energies of Two Interstitial Configurations in a Face-Centered Cubic Crystal

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The energies of formation for two configurations of an interstitial in a face-centered cubic crystal were calculated. One interstitial was in the body-centered position and the other is formed by two atoms sharing and slightly displaced from a normal face-center site. A Morse potential function for copper was used for the interaction between the atoms. The results of this calculation indicate that the energies of formation differ by a small fraction of an electron volt.

## I. INTRODUCTION

THE energy of formation of an interstitial defect in a crystal depends upon the geometry of the defect. In an effort to decide which of two different configurations is energetically preferred, the energy of formation and the equilibrium configuration of each were determined. The two geometries, described below, have the greatest expectation of being stable because they both make use of the large "open space" in the center of the lattice cube and because they contain the largest number of symmetry elements. The calculations reported here are an attempt to compare the relative energies of formation of the two interstitial configurations using a pairwise potential, such as the Morse potential, with the results from other methods in which the ion-core repulsive potential and the attractive potential due to the conduction electrons are treated separately.

Huntington[1] calculated the energy of formation of an interstitial in a body-centered position of a face-centered cubic crystal and of an interstitial in a position in which the interstitial and another atom are arranged symmetrically about a face center on a line perpendicular to the face. His results indicated that the latter split interstitial configuration had an energy of formation about 0.25 eV lower than the other.

In a study of a copper-crystal model through which copper atoms were fired, Gibson *et al.*[2] found that if the interatomic potential is represented by a suitable Born-Mayer potential, the extra atom always comes to rest in the split configuration. Static calculations, which like the dynamic ones did not force a symmetry on the interstitial structure, showed that the split configuration is preferred and that the body-centered configuration is not stable.

Using a Born-Mayer potential, Bennemann[3,4] has calculated the contribution of the pairwise forces to the energy of formation of the split configuration to be 3.548 eV. The calculation treated the region outside the region of moving atoms as an elastic continuum.

Our calculation does not minimize the sum of electron redistribution and pairwise energies. Instead, the equilibrium configurations and energies using the pairwise force alone were calculated in a small cluster of movable atoms inside a rigid lattice. The elastic region-energy contribution was neglected.

## II. METHOD OF CALCULATION

The formation energy of an interstitial is the sum of the energies obtained by (1) placing an atom in an unrelaxed crystal in an arbitrary starting position, (2) allowing the crystal to relax about the defect, and (3) removing an atom from the surface of the crystal so as to end with the same number of atoms as at the start.

Calculation of the relaxation energy in step (2) is the main problem. The method used was to minimize the interaction energy $E$ of a cube of face-centered array ten lattice units on a side containing about 4630 normal atoms and one interstitial. The origin of the coordinate system was taken as the interstitial in the body-centered case and as the empty lattice site between the two displaced atoms in the split interstitial case. The unit of length was taken as one-half the lattice parameter. This allowed lattice sites in the perfect, unrelaxed crystal to have integral values of coordinates.

In both cases, groups of atoms with the same symmetry relative to the interstitial were required to carry out their relaxation in a symmetric manner. The relaxation was represented by the three components of the displacement of an atom away from its normal lattice site, hereafter called position variables ($\Delta_1$, $\Delta_2$, and $\Delta_3$). Three of these describe the motion of a set of atoms; one or two of these could be zero and two or three could be equal as a result of the symmetry requirement. The atoms within a sphere of approximate radius$=(13)^{1/2}$ were allowed to move. For the body-centered interstitial eleven different position variables sufficed to describe the motion of the 117 atoms nearest the defect. In the split configuration, reduced symmetry required the use of 22 position variables to represent the motion of 88 atoms. The rest of the atoms remained fixed.

The computer program varied the position variables of the system in order to find a minimum of $E$ which has the form

$$E=\tfrac{1}{2}\sum_{i\neq j}\varphi(r_{ij})+\sum_{i,k}\varphi(r_{ik}). \quad (1)$$

[1] H. B. Huntington, Phys. Rev. **91**, 1093 (1953).
[2] J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, Phys. Rev. **120**, 1229 (1960).
[3] K. H. Bennemann, Phys. Rev. **124**, 669 (1961).
[4] K. H. Bennemann, Z. Physik **165**, 445 (1961).

TABLE I. Position variables of atoms near the body-centered interstitial.

| Coordinates of displaced atom | $\Delta_1=\Delta x/1.804$Å | $\Delta_2=\Delta y/1.804$Å | $\Delta_3=\Delta z/1.804$Å |
|---|---|---|---|
| 001 | 0 | 0 | 0.2222 |
| 111 | −0.0128 | −0.0128 | −0.0128 |
| 012 | 0 | 0.0359 | 0.0415 |
| 221 | 0.0022 | 0.0022 | 0.0085 |
| 003 | 0 | 0 | −0.0093 |
| 023 | 0 | 0.0120 | 0.0101 |
| 113 | 0.0038 | 0.0038 | 0.0088 |

Here $i$ and $j$ range over the atoms free to move and $k$ ranges over the nonmoving atoms. $\varphi$ is a Morse function calculated by Girifalco and Weizer[5] using the observed lattice parameter, the cohesive energy, and the compressibility of copper. It has the form

$$\varphi(r_{ij})=D\{\exp[-2\alpha(r_{ij}-r_0)] -2\exp[-\alpha(r_{ij}-r_0)]\}, \quad (2)$$

where $r_{ij}$ is the distance between the $i$th and $j$th atoms, $D$ is equal to 0.3429 eV, $\alpha$ is equal to 1.3588Å$^{-1}$ and $r_0$ is 2.866Å. The difference between the minimum $E$ and $E_0$, the value of $E$ in the arbitrary starting position, is the relaxation energy.

## III. RESULTS AND DISCUSSION

The energies of formation were calculated by the relaxation program to be 4.55 eV for the body-centered configuration and 4.54 eV for the split configuration. The position variables for the relaxed configurations are given in Tables I and II. The negative sign denotes displacement from the normal-lattice site in the direction of decreasing the magnitude of the coordinate. The units used are one-half the lattice parameter or 1.80 Å. The axis of the split configuration is parallel to the $z$ axis.

TABLE II. Position variables of atoms near the split interstitial.

| Coordinates | $\Delta_1=\Delta x/1.804$Å | $\Delta_2=\Delta y/1.804$Å | $\Delta_3=\Delta z/1.804$Å |
|---|---|---|---|
| 000 | 0 | 0 | 0.5809 |
| 101 | 0.1368 | 0 | −0.0725 |
| 110 | −0.0468 | −0.0468 | 0 |
| 002 | 0 | 0 | −0.0113 |
| 200 | 0.0097 | 0 | 0 |
| 112 | 0.0084 | 0.0084 | 0.0074 |
| 211 | 0.0123 | 0.0210 | −0.0055 |
| 202 | 0.0350 | 0 | 0.0338 |
| 220 | −0.0058 | −0.0058 | 0 |
| 222 | 0.0035 | 0.0035 | 0.0053 |
| 103 | −0.0020 | 0 | −0.0049 |
| 301 | −0.0044 | 0 | 0.0017 |
| 310 | 0.0067 | −0.0005 | 0 |

The Morse potential used in this calculation represents the effect of the conduction electrons by a pairwise long-range attractive term. However, the energy of the conduction electrons depends on the wave covering the entire crystal and is better represented by a term related to the volume of the crystal. Since the two energies of formation calculated on the basis of the pairwise forces are equal, the preferred configuration must be determined on the basis of electron redistribution corrections.

[5] L. A. Girifalco and V. G. Weizer, J. Phys. Chem. Solids **12**, 260 (1960).