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VACANCY BEHAVIOR IN A COMPRESSED

fcc LENNARD-JONES CRYSTAL

by

Joe R. Beeler, Jr.

ABSTRACT

This computer experiment study concerns the determination of the stable vacancy configuration in a compressed fcc Lennard-Jones crystal and the migration of this defect in a compressed crystal. Isotropic and uniaxial compression stress conditions were studied. The isotropic and uniaxial compression magnitudes employed were $0.94 \leq \eta \leq 1.5$, and $1.0 \leq \eta \leq 1.5$, respectively. The site-centered vacancy (SCV) was the stable vacancy configuration whenever cubic symmetry was present. This includes all of the isotropic compression cases and the particular uniaxial compression case ($\eta = \sqrt{2}$) that give a bcc structure. In addition, the SCV was the stable configuration for uniaxial compression $\eta < 1.29$. The out-of-plane split vacancy (SV-OP) was the stable vacancy configuration for uniaxial compression $1.29 < \eta \leq 1.5$ and was the saddle-point configuration for SCV migration when the SCV was the stable form. For $\eta > 1.20$, the SV-OP is an extended defect and, therefore, a saddle point for SV-OP migration could not be determined. The mechanism for the transformation from the SCV to the SV-OP as the stable form at $\eta = 1.29$ appears to be an alternating sign $[101]$ and/or $[011]$ shear process.

I. INTRODUCTION

This report describes computational results for the static equilibrium properties of a vacancy in a compressed face-centered cubic (fcc) Lennard-Jones crystal as a function of compression. The static equilibrium properties calculated were the displacement fields and configuration energies for a site-centered vacancy (SCV) and a split vacancy (SV). These two vacancy configurations are described in Fig. 1. An SCV is produced by removing an atom from a normal atom

Fig. 1a.
Site-centered vacancy (SCV) at
site A.

Fig. 1b.
Split vacancy (SV) consisting
of an atom located midway be-
tween unoccupied sites A and B.

site A in a crystal. An SV is produced by first creating an SCV at site A and then moving the atom at one of the first-neighbor sites B of A to the point midway between A and B. Two cases were considered: (1) uniaxial compression along the [001] direction and (2) isotropic compression. The compression (η) ranges considered were $1.0 \leq \eta \leq 1.5$, for uniaxial compression, and $0.97 \leq \eta \leq 1.5$ for isotropic compression. The calculations were done using the MOLDY program, a dynamical method computer experiment program written by B. L. Holian and G. K. Straub. A dynamical method program can be modified to compute static equilibrium properties of defects by adding a velocity damping term to the equations of motion. This modification was made in the MOLDY program to provide a capability for doing defect static equilibrium property calculations. Detailed explanations and illustrations of how to perform static equilibrium computations for defects in bcc, fcc, and hcp crystals are given by Beeler (1970) and by Beeler and Beeler (1979a, b, c, d).

The present study was suggested by B. L. Holian and was made for the purpose of gaining background data for use in the interpretation of mass transport results obtained in dynamical method computer experiments on shock processes in an fcc Lennard-Jones crystal containing vacancy defects. These shock process simulations will be made using the MOLDY program. Guinan et al. (1977) showed that most of

the dynamical attributes of interstitial diffusion in tungsten(m3),* observed in a fully dynamical simulation of interstitial migration in tungsten(m3), could be inferred from static equilibrium calculations of the displacement fields and configuration energies for the stable interstitial and interstitial migration saddle-point configurations. This particular experience indicated that static equilibrium calculations for the displacement fields and configuration energies for the stable vacancy and the vacancy migration saddle-point configurations in a compressed crystal should give valuable data for use in interpreting the results of dynamical method shock wave simulations for crystals containing vacancy defects.

In particular, one might expect that the migration energy for vacancy movement parallel to the uniaxial stress axis would differ significantly from that for vacancy movement perpendicular to the stress axis. In addition, one might expect that the displacement field details for vacancy movement during uniaxial compression would differ significantly from those for vacancy movement during isotropic compression. In this regard, one might expect that experimental data for defect motion obtained in hydrostatic pressure experiments need not be applicable in analyzing the results of shock wave experiments. The results described in this report confirm these particular expectations for face-centered tetragonal (fct) and fcc Lennard-Jones crystals.

It was found that the stable vacancy configuration changes from an SCV to an SV at compression $\eta = 1.29$ during uniaxial compression. This vacancy configuration change is a new result that has not been reported previously. In the case of isotropic compression, however, the SCV configuration is stable up to $\eta = 1.5$. No calculations were done for $\eta > 1.5$.

II. INTERATOMIC POTENTIAL AND COMPUTATIONAL CELL

The Lennard-Jones atom pair potential energy function used was

$$V(r) = \epsilon \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^6 \right] , \quad (1)$$

*Tungsten(m3) is a model for tungsten metal, which consists of joining the Wilson and Bisson (1971) tungsten potential with the Johnson and Wilson (1972) tungsten potential at about 1.7 Å, with the Wilson-Bisson potential being used for atom separation distances less than 1.7 Å. The Wilson-Bisson and Johnson-Wilson potentials are referred to as tungsten(m1) and tungsten(m2), respectively.

where $r_0 = 3.8666 \text{ \AA}$ and $\epsilon = 9.10858 \times 10^{-3} \text{ eV}$. This potential was truncated to $V(r) = 0$ at $r_{\text{cut}} = 7.486592 \text{ \AA}$.

The MOLDY computational cell used was a 500-site fcc crystallite with periodic boundary conditions. The cell was a cube with $\{100\}$ faces in the case of isotropic compression and a right rectangular parallelepiped with $\{100\}$ faces in the case of uniaxial compression. In each case there were five unit cells along each Cartesian coordinate axis, each of which contained four atoms. This gives a total of 125 unit cells and 500 atom sites. For compression $\eta = 1.0$, the lattice constant was $a_0 = 5.468198 \text{ \AA}$. For uniaxial compression, the lattice constant along each of the directions $[100]$ and $[010]$ was a_0 ; but that along the $[001]$ direction was a_0/η , giving an fct crystal. An xy-plane in the fct crystal, in which the lattice constant along both $[100]$ and $[010]$ is a_0 for all η , will be called a basal plane. The basal plane half-lattice constant will be denoted as $\text{hlc}(xy)$ and is equal to $a_0/2$. The half-lattice constant along the z-axis will be denoted as $\text{hlc}(z)$ and is equal to $a_0/2\eta$. For isotropic compression the lattice constant was $a_0/(\eta)^{1/3}$ for each of the three coordinate directions.

Atom site number and atom site coordinate maps for the 500-site computational cell are given in Fig. 2. Figure 2a is an xy-plane map, which is applicable for each odd-numbered (NZ) plane, and Fig. 2b is an xy-plane map, which is applicable for each even-numbered (NZ) plane. The atom site coordinates are expressed in hlc and $\text{hlc}(xy)$ for the x- and y-directions and $\text{hlc}(z)$ for the z-direction. The appropriate plane number (NZ), plane z-coordinate (z), and site number (NS) range for each plane concerned are listed in a guide table located at the right side of each map. Given the coordinates (x,y,z) of an atom site, S, one can find the associated computational cell site number, NS, in two steps: (1) use the z-coordinate to select the proper map section (the map section whose guide table lists the z-coordinate concerned), (2) use (x,y) to locate site S on the map. At the site location (x,y) the map gives an integer label L. The associated site number NS is given by

$$NS = 100 \frac{NZ - 1}{2} + L \quad (\text{for odd NZ}), \quad (2a)$$

$$NS = 100 \frac{NZ - 2}{2} + L \quad (\text{for even NZ}). \quad (2b)$$

Fig. 2.

Atom site number and site coordinate maps for a MOLDY program 500-site fcc computational cell.

When an fcc crystal is compressed uniaxially along the [001] direction, from $\eta = 1.0$ to $\eta = \sqrt{2}$, the crystal structure changes from fcc, at $\eta = 1.0$, to bcc at $\eta = \sqrt{2}$. This change is described in Fig. 3. Figure 3a shows the atom sites in two adjacent fcc cubic unit cells. The unit of length is an hlc; hence, the edge length of the cubic unit cell is 2.0. Atom sites represented by open circles lie in the $x = 0$ plane, those represented by filled circles lie in the $x = 1.0$ plane, and those represented by hatched circles lie in the $x = 2.0$ plane. Note that the sites numbered 1-8 are at the corners of the right parallelepiped with a square base, and that site 9 is located at the center of this parallelepiped. The height of the parallelepiped is 2.0 and the edge length of its square base is $\sqrt{2}$. Figure 3b shows sites 1-9 only and ignores the other sites depicted in Fig. 3a. Figure 3b defines a tetragonal unit cell for an fcc crystal and contains two atoms, one-eighth of an atom at each of the eight corners and one atom at the center of the cell. It is clear that a uniaxial compression $\eta = \sqrt{2}$ along the [001] direction reduces the parallelepiped of height 2.0, shown in Fig. 3b, to the cube of edge length $\sqrt{2}$, shown in Fig. 3c. One recognizes Fig. 3c as being a cubic unit cell for a bcc crystal. This bcc unit cell contains two atoms, one-eighth of an atom at each of the eight corners and one atom at the center of the cell.

One can use Figs. 3b and 3c to relate the direction of a line segment connecting the centers of two given atoms in the fcc cell, at $\eta = 1.0$, to the direction of the line segment connecting the centers of these same two atoms in the bcc cell at $\eta = \sqrt{2}$. For example, the direction from site 9 to site 3 in the fcc cell (Fig. 3b) is [101]. Figure 3 shows that the direction from site 9 to site 3 in the bcc cell is [111]. Hence, $[101]_{\text{fcc}}$ goes into $[111]_{\text{bcc}}$. Table I lists site-to-site line segments and the corresponding directions for these segments in the fcc cell and the bcc cell. Perhaps the most important of these correspondences are (1) $[100]_{\text{fcc}}$ goes into $[110]_{\text{bcc}}$, (2) $[010]_{\text{fcc}}$ goes into $[\bar{1}10]_{\text{bcc}}$, and (3) $[001]_{\text{fcc}}$ goes into $[001]_{\text{bcc}}$.

Table II lists the relative coordinates RC_n and coordination number CN_n for sites in each of the first ten neighbor shells of a given site S in an fcc crystal and in a bcc crystal. Given a site S with coordinates (x,y,z) , and a neighboring site S' with coordinates (x',y',z') , the relative coordinates of S' with respect to S are $x_r = (x' - x)$, $y_r = (y' - y)$, and $z_r = (z' - z)$. In terms of relative coordinates, any given neighbor shell may consist of two or more subshells, each corresponding to a different set of relative coordinates. For

(a) Two cubic unit cells for an fcc crystal ($\eta = 1.0$).

(b) A tetragonal unit cell for an fcc crystal ($\eta = 1.0$).

(c) A cubic unit for a bcc crystal obtained by uniaxial compression $\eta = \sqrt{2}$ of the fcc cell in (b) along $[001]$.

Fig. 3.

Transition from an fcc crystal to a bcc crystal via uniaxial compression along $[001]$.

TABLE I

Correspondence between the direction of a site-to-site segment in the fcc crystal ($\eta = 1.0$) and that for this segment in the bcc crystal occurring at $\eta = \sqrt{2}$. Site numbers defined in Fig. 3.

Site-to-Site Segment	Direction	
	fcc Crystal ($\eta = 1.0$)	bcc Crystal ($\eta = \sqrt{2}$)
1 to 3	[100]	[110]
4 to 2	[010]	[$\bar{1}$ 10]
5 to 1	[001]	[001]
1 to 4	[$\bar{1}$ 10]	[200]
1 to 2	[110]	[020]
5 to 1	[001]	[001]
9 to 3	[101]	[111]
9 to 2	[011]	[$\bar{1}$ 11]
9 to 1	[$\bar{1}$ 01]	[$\bar{1}$ $\bar{1}$ 1]
9 to 4	[0 $\bar{1}$ 1]	[1 $\bar{1}$ 1]
9 to 7	[10 $\bar{1}$]	[11 $\bar{1}$]
9 to 6	[01 $\bar{1}$]	[$\bar{1}$ 1 $\bar{1}$]
9 to 5	[$\bar{1}$ 0 $\bar{1}$]	[$\bar{1}$ $\bar{1}$ $\bar{1}$]
9 to 8	[0 $\bar{1}$ $\bar{1}$]	[11 $\bar{1}$]

example, the sum of the squares of the relative coordinates for a site in the 10th neighbor shell in a bcc crystal is 27, i.e., $r_{10}^2 = 27$. There are two relative coordinate sets which give $r_{10}^2 = 27$; one is $(\pm 3, \pm 3, \pm 3)$ and the other is $(\pm 5, \pm 1, \pm 1)$. Also given in Table II is the ratio r_n/r_1 of the n -th neighbor shell radius to the radius r_1 of the first neighbor shell. This ratio can be used to determine from what initial fcc subshell each member of a bcc subshell evolved during uniaxial compression from $\eta = 1.0$ to $\eta = \sqrt{2}$.

Table III gives the neighbor subshell transformation correspondence for going from an fcc crystal ($\eta = 1.0$) to a bcc crystal ($\eta = \sqrt{2}$) via uniaxial compression along the [001] direction.

This table was prepared to show how

each of the first six neighbor shells in the bcc crystal evolved from particular subshells in the fcc crystal.

One procedure for constructing Table III is as follows. At uniaxial compression $\eta = \sqrt{2}$, $\text{hlc}(\text{xy}) = \sqrt{2}\text{hlc}(\text{bcc})$, $\text{hlc}(\text{bcc})$ being the bcc crystal half-lattice constant. From Table I or from Fig. 3, it follows that, at this compression, $[100]_{\text{fcc}}$ is coaxial with $[110]_{\text{bcc}}$, $[010]_{\text{fcc}}$ is coaxial with $[$\bar{1}$ 10]_{\text{bcc}}$, and $[001]_{\text{fcc}}$ is coaxial with $[001]_{\text{bcc}}$. Hence, a unit distance of one $\text{hlc}(\text{xy})$ along $[100]_{\text{fcc}}$ is equal to a distance of $\sqrt{2}\text{hlc}(\text{bcc})$ along $[110]_{\text{bcc}}$, a distance of one $\text{hlc}(\text{xy})$ along $[010]_{\text{fcc}}$ is equal to a distance of $\sqrt{2}\text{hlc}(\text{bcc})$ along $[$\bar{1}$ 10]_{\text{bcc}}$, and one $\text{hlc}(z)$ along $[001]_{\text{fcc}}$ is equal to one $\text{hlc}(\text{bcc})$ along $[001]_{\text{bcc}}$. This demonstrates that the vectors $[100]_{\text{fcc}}$ and $[110]_{\text{bcc}}$ are equal, as are the vectors $[010]_{\text{fcc}}$ and $[$\bar{1}$ 10]_{\text{bcc}}$ and the vectors $[001]_{\text{fcc}}$ and $[001]_{\text{bcc}}$. Consequently, the vector $\mathbf{r}_r = (x_r, y_r, z_r)$ from S to S' in the fct coordinate system is

$$r_r(\text{fct}) = x_r[100]_{\text{fct}} + y_r[010]_{\text{fct}} + z_r[001]_{\text{fct}} \quad (3a)$$

$$= x_r[110]_{\text{bcc}} + y_r[\bar{1}10]_{\text{bcc}} + z_r[001]_{\text{bcc}} \quad (3b)$$

In the bcc coordinate system, this vector is, from Eq. (3b),

$$r_r(\text{bcc}) = (x_r - y_r)[100]_{\text{bcc}} + (x_r + y_r)[010]_{\text{bcc}} + z_r[001]_{\text{bcc}} \quad (4)$$

TABLE II

Neighbor shell relative coordinates RC_n , radius r_n , and coordination number C_n for each of the first ten neighbor shells in an fcc and a bcc crystal. The relative coordinates are expressed in half-lattice constants (hlc). n is the neighbor shell number (index).

fcc Crystal Neighbors				bcc Crystal Neighbors			
<u>n</u>	<u>RC_n</u>	<u>r_n^2</u>	<u>C_n</u>	<u>n</u>	<u>RC_n</u>	<u>r_n^2</u>	<u>C_n</u>
1	(1,1,0)	2	12	1	(1,1,1)	3	8
2	(2,0,0)	4	6	2	(2,0,0)	4	6
3	(2,1,1)	6	24	3	(2,2,0)	8	12
4	(2,2,0)	8	12	4	(3,1,1)	11	24
5	(3,1,0)	10	24	5	(2,2,2)	12	8
6	(2,2,2)	12	8	6	(4,0,0)	16	6
7	(3,2,1)	14	48	7	(3,3,1)	19	24
8	(4,0,0)	16	6	8	(4,2,0)	20	24
9	(3,3,0)	18	12	9	(4,2,2)	24	24
10	(4,1,1)	18	24	10	(3,3,3)	27	8
10	(4,2,0)	20	24	10	(5,1,1)	27	24

<u>n</u>	<u>r_n/r_i</u>	<u>n</u>	<u>r_n/r_i</u>
1	1.0	1	1.0
2	1.4142	2	1.1547
3	1.732	3	1.6330
4	2.0	4	1.9148
5	2.2361	5	2.0
6	2.4495	6	2.3094
7	2.6458	7	2.5166
8	2.8284	8	2.5820
9	3.0	9	2.8284
10	3.1623	10	3.0

TABLE III

Neighbor subshell transformation correspondence in going from an fcc crystal ($\eta = 1.0$) to a bcc crystal ($\eta = \sqrt{2}$) by means of uniaxial compression along the [001] direction.

fcc Crystal			bcc Crystal		
Number of Sites	Subshell Type	Shell No.	Number of Sites	Subshell Type	Shell No.
8	<101>	1	8	<111>	1
4	<110>	1	4	<200>	2
2	<002>	2	2	<002>	2
4	<200>	2	4	<220>	3
8	<112>	3	8	<202>	3
16	<121>, <211>	3	16	<311>	4
8	<103>	5	8	<113>	4
8	<202>	4	8	<222>	5
4	<220>	4	4	<400>	6
2	<004>	8	2	<004>	6

Relations (3) and (4) show that the relative coordinates (x_r, y_r, z_r) in the fcc crystal transform to bcc crystal relative coordinates, at $\eta = \sqrt{2}$, as follows:

$$x_r(\text{bcc}) = (x_r - y_r) \quad , \quad (5a)$$

$$y_r(\text{bcc}) = (x_r - y_r) \quad , \quad (5b)$$

$$z_r(\text{bcc}) = z_r \quad . \quad (5c)$$

Table III also can be constructed by computing the distance between a site S and each of its neighbors after uniaxial compression $\eta = \sqrt{2}$ along [001] and taking the ratio of this distance to $r_1(\text{bcc})$. Because there is a unique value of r_n/r_1 for each neighbor shell n, the distance ratio obtained indicates the proper neighbor shell in the bcc crystal. Let (x_r, y_r, z_r) be the relative coordinates of site S' with respect to site S when $\eta = 1.0$. The distance from S to S' is then

$$d(\text{S to S}') = (x_r^2 + y_r^2 + z_r^2/\eta^2)^{1/2} \quad , \quad (6)$$

$$d(\text{S to S}') = (x_r^2 + y_r^2 + z_r^2/2.0)^{1/2} \quad , \quad \eta = \sqrt{2} \quad . \quad (7)$$

From Fig. 3c, the bcc first neighbor distance $r_1(\text{bcc})$ is the length of the site-to-site segment from site 9 to site 3. Using Eq. (7) one obtains $r_1(\text{bcc}) = 1.224745$ and the unit of length is $hlc(xy)$. As an example, consider the fcc first neighbor subshell whose relative coordinates are $(\pm 1, 0, \pm 1)$. For each of these neighbors $d(S \text{ to } S') = 1.224745$ when $\eta = \sqrt{2}$, and, hence, each of them also is a first neighbor in the bcc crystal. In contrast, the sites in the $(\pm 1, \pm 1, 0)$ fcc first neighbor subshell give $d(S \text{ to } S') = 1.414214$ when $\eta = \sqrt{2}$. This gives a ratio $d(S \text{ to } S')/r_1 = 1.154701$. According to Table II this ratio indicates the second neighbor shell in the bcc crystal.

III. PERFECT CRYSTAL ENERGY

The perfect crystal energy is plotted in Fig. 4a as a function of compression. The upper curve is for uniaxial compression and the lower curve is for isotropic compression. The data base for these plots is given by Tables IV and V. In the case of uniaxial compression, the lowest energy occurred for $\eta = 1.10$ (see Table IV). The lowest energy occurred near $\eta = 1.10$ in the case of isotropic compression. A blowup of the crystal energy for isotropic compression (Fig. 4b) shows a relative minimum at $\eta = 1.06$ and a discontinuity at $\eta = 1.102$ (see Appendix A). This discontinuity is caused by the truncation of the potential function at the atom separation distance $r_{\text{cut}} = 7.486592 \text{ \AA}$. For $\eta < 1.1021107$, each atom interacts only with its first, second, and third neighbors. At $\eta = 1.1021107$, interaction with fourth neighbors occurs, in addition, and causes the sharp drop pictured in Fig. 4a. As indicated in Table I, there are 12 fourth neighbors. A second discontinuity would occur at $\eta = 1.540250$ due to the addition of fifth neighbor interactions. There are 24 fifth neighbors, as indicated in Table I.

Discontinuities also occur in the crystal energy curve for uniaxial compression at $\eta = 1.0694$, 1.1769 , and 1.4608 but are not detectable in Fig. 4a because the density of data points is too sparse to reveal them. The first of these discontinuities is caused by the addition of $[202]$ and $[022]$ fourth neighbor interactions which involve eight of the twelve fourth neighbors. The second discontinuity is caused by additional interactions with $[103]$ and $[013]$ fifth neighbors which involve only 8 of the 24 fifth neighbors. The third discontinuity is caused by the addition of two $[004]$ eighth neighbors. The neighbor shell reference used here for the additional interaction atoms denotes the shells in which the particular atoms concerned are located when $\eta = 1.0$.

Fig. 4.

- (a) Crystal energy vs compression for uniaxial and isotropic compression of an fcc Lennard-Jones crystal.
- (b) Blowup of the crystal energy for isotropic compression in the neighborhood of the energy discontinuity at $\eta = 1.1021107$.

TABLE IV

Crystal energy $E^X(\text{PC})$ for a perfect 500-atom fcc crystal obtained by uniaxial compression of a 500-atom fcc Lennard-Jones crystal along [001].

Compression	$E^X(\text{PC}), \text{eV}$	$E^A(\text{PC}), \text{eV}$
1.0	-34.490068	-0.068980
1.05	-34.789679	0.069579
1.10	-34.984722	-0.069969
1.15	-33.604673	-0.067209
1.20	-31.994802	-0.063990
1.25	-28.768570	-0.057537
1.30	-24.494780	-0.048990
1.33..	-21.042101	-0.042084
1.375	-16.016528	-0.032033
1.40	-12.040060	-0.024080
1.414..	-10.524629	-0.021049
1.45	-4.815714	-0.009631
1.50	4.205555	-0.008411

TABLE V

Crystal energy $E^X(\text{PC})$ for a perfect 500-atom fcc crystal obtained by isotropic compression of a 500-atom fcc Lennard-Jones crystal.

Compression	$E^X(\text{PC}), \text{eV}$	$E^A(\text{PC}), \text{eV}$
0.9703	-33.992791	-0.067986
1.0	-34.490068	-0.068980
1.0303	-34.809020	-0.069618
1.05	-34.905721	-0.069811
1.0612	-34.919161	-0.069838
1.07	-34.908016	-0.069816
1.0927	-34.786729	-0.069573
1.10	-34.718546	-0.069437
1.11	-35.642621	-0.071285
1.1249	-35.442990	-0.070886
1.13	-35.359072	-0.070718
1.15	-34.956531	-0.069913
1.1910	-33.733827	-0.067008
1.20	-33.390618	-0.066001
1.2250	-32.282121	-0.064564
1.25	-30.945933	-0.061892
1.2597	-30.360609	-0.060721
1.30	-27.521446	-0.055043
1.3310	-24.859952	-0.049720
1.33	-24.642028	-0.049284
1.375	-20.315167	-0.040630
1.40	-17.306071	-0.034612
1.45	-10.291589	-0.020583
1.50	-1.849878	-0.003700

Table VI gives the number of atom pair interactions (NPI) per atom as a function of compression. The calculations involved are given in Appendix A. NPI is constant over most of the range of interest, $1.102 < \eta \leq 1.5$, for isotropic compression. For uniaxial compression, NPI is constant over a slightly smaller range, $1.177 < \eta < 1.46$. Within these two compression ranges there are no discontinuities in the crystal energy.

TABLE VI

The number of atom pair interactions (NPI) per atom as a function of compression.

(a) NPI for Selected Compression Values

η	Uniaxial Compression	Isotropic Compression
1.0	42	42
1.05	42	42
1.10	50	42
1.15	50	54
1.20	58	54
1.25	58	54
1.30	58	54
1.33	58	54
1.375	58	54
1.40	58	54
1.414	58	54
1.45	58	54
1.50	60	54

(b) NPI for Compression Ranges

Uniaxial Compression	NPI
$1.0 \leq \eta < 1.069365$	42
$1.069365 \leq \eta < 1.176887$	50
$1.176887 \leq \eta < 1.460798$	58
$1.460798 \leq \eta \leq 1.50$	60
<hr/>	
Isotropic Compression	NPI
$1.0 \leq \eta < 1.102111$	42
$1.102111 \leq \eta \leq 1.5$	54

IV. VACANCY CONFIGURATION AND RELAXATION ENERGY

A. Introduction

The configuration energy $E^C(D)$ for a particular defect D is defined as

$$E^C(D) = E^X(D) - E^X(PC) \quad , \quad (8)$$

where $E^X(PC)$ is the energy of the perfect crystal configuration and $E^X(D)$ is the energy of the crystal after the defect configuration has been established in the crystal. In the case of a vacancy, $E^X(D)$ is the crystal energy obtained when an atom is extracted from a normal atom site and all other atoms are allowed to change their positions in response to any unbalanced forces introduced by the extraction. Atom positional change occurring as a result of introducing a defect is called relaxation. In general, introduction of a defect involves (1) an initial removal and/or creation of atom pair interactions, and (2) a consequent relaxation of atom positions. The defect configuration energy obtained when only the initial atom pair interaction changes are accounted for and relaxation is not considered, is called the unrelaxed configuration energy $E^C(D)_{ur}$. The difference,

$$E^R(D) = E^C(D)_{ur} - E^C(D) \quad , \quad (9)$$

between $E^C(D)_{ur}$ and $E^C(D)$ is called the relaxation energy of the defect.

The magnitude of the relaxation energy relative to that of the unrelaxed configuration energy reflects the intensity of the relaxation process for a given defect. In this context, the relaxation intensity $I_r(D)$ for a defect D will be defined as

$$I_r(D) = \left| E^R(D) / E^C(D)_{ur} \right| \quad . \quad (10)$$

The migration energy $E^m(D)$ for a particular defect D is defined as

$$E^m(D) = E^X(SP) - E^X(D) \quad , \quad (11)$$

where $E^X(SP)$ is the crystal energy when the saddle-point configuration for defect D migration has been introduced. Determination of the saddle-point configuration

for defect migration is discussed in detail by Beeler and Beeler (1979d). In computer experiment work, an estimate of the vacancy formation energy $E^f(V)$ commonly is obtained using the recipe

$$E^f(V) = E^c(V) + E^a(PC) , \quad (12)$$

where $E^a(PC)$ is the potential energy per atom (cohesive energy) for a perfect crystal. $E^c(V)$ is the increase in the crystal energy which occurs when an atom is removed from a normal site in a perfect crystal. $E^a(PC)$ is the decrease in crystal energy which occurs when the removed atom is relocated on the crystal surface at an interior corner in a surface ledge. The rationale for this recipe is discussed by Damask and Dienes (1963). Hirth (1972) gives a careful theoretical discussion of the considerations involved in a defect-formation energy computation. In the case of an SCV,

$$E^c(V)_{ur} = -2E^a(PC) , \quad (13)$$

and, from Eq. (9),

$$E^r(V) = E^c(V)_{ur} - E^c(V) . \quad (9)$$

Relations (9) and (13), together with (12), give

$$E^f(SCV) = -[E^a(PC) + E^r(SCV)] \quad (14)$$

for an SCV. For an SV, one has

$$E^r(SV) = E^c(SV) - E^r(SV) + E^a(PC) . \quad (15)$$

As mentioned previously, an fcc crystal that is subjected to uniaxial compression η along the [001] direction becomes an fct crystal with lattice constant a along the [100] and [010] directions and lattice constant $c = a/\eta$ along the [001] direction. Two types of atom migration occur in a tetragonal crystal. One of these is atom migration in a basal plane, called in-plane migration, and

the other is that in which an atom moves from one basal plane to another adjacent basal plane, called out-of-plane migration. Similarly, there are two kinds of split vacancies in a tetragonal crystal, the in-plane split vacancy, SV-IP, and the out-of-plane split vacancy, SV-OP. The present work indicates that the stable vacancy configuration is the SCV for uniaxial compression $\eta < 1.29$, and changes to the SV-OP for $\eta > 1.29$.

When the SCV is the stable configuration, in-plane migration in a tetragonal crystal with a [001] tetragonal axis proceeds as shown schematically in Figs. 5a, b, and c. One of the first-neighbor atoms, B, of the initially vacant site A, moves to site A, thereby filling the original vacancy and leaving a vacancy at site B. The saddle-point configuration is the SV-IP shown in Fig. 5b. In this instance the crystal energy change profile versus the moving atom position r_c on the reaction coordinate line between sites A and B has a single peak at r_c^* midway between A and B, as shown in Fig. 6a.

Out-of-plane migration of an SCV in a tetragonal crystal with a [001] tetragonal axis involves a first-neighbor atom at a site B in an adjacent basal plane moving into the initially vacant site A. In this instance the saddle point can be either simple or complex. In the simple case the saddle-point configuration is the SV-OP shown in Fig. 5d, and the associated crystal energy change profile is like that shown in Fig. 6a. A pair of saddle-point configurations exists, in the complex case, wherein the moving atom is positioned a distance d^* on either side of the midpoint. The crystal energy change profile versus r_c exhibits two peaks; one at r_1^* and the other at r_2^* , as shown in Fig. 6b. The distance from the midpoint to either r_1^* or r_2^* is d^* . The valley between the two peaks normally is shallow, being only about 4% of the peak height. Because of this standard result for a twin-peak saddle point, the crystal energy for the SV-OP midpoint configuration can be used as an estimate of the crystal energy for the saddle-point configuration. A detailed account of how to compute complete crystal energy profiles, such as those shown in Fig. 6, is given by Beeler and Beeler (1979d).

When the SV-OP is the stable vacancy configuration, the saddle-point configuration probably is complex. A schematic description of the crystal energy change profile for SV-OP migration is given in Fig. 7. This figure is based on the assumption that the SCV is the midpoint configuration. Past experience indicates that $E^C(\text{SP})$ should be only slightly larger than $E^C(\text{SCV})$.

Fig. 5.

(a), (b), and (c) show migration of an SCV from site A to site B. The SV in (b) is the saddle-point configuration. This sequence pertains either to SCV migration in an fcc crystal or to SCV migration in a basal plane of an fct crystal. An out-of-plane split vacancy (SV-OP) in an fct crystal is shown in (d). An in-plane split vacancy (SV-IP) in an fct crystal is shown in (b).

Fig. 6a.

Crystal energy profile for SCV migration in the case of a simple saddle-point configuration.

Fig. 6b.

Crystal energy profile for SCV migration in the case of a complex saddle-point configuration.

Fig. 7.

Configuration energy profile for SV migration.

SP = SADDLE POINT

SCV = SITE-CENTERED VACANCY

SV = SPLIT-VACANCY

B. Vacancy Configuration and Relaxation Energy

1. Site-Centered Vacancy. The SCV configuration energy is plotted in Fig. 8 as a function of compression. The upper curve pertains to isotropic compression and the lower curve to uniaxial compression. In the case of isotropic compression, $E^C(\text{SCV})$ is positive for $\eta < 1.46$ and negative for $1.46 \leq \eta \leq 1.5$. For uniaxial compression, $E^C(\text{SCV})$ is positive for $\eta < 1.27$ and negative for $1.27 \leq \eta \leq 1.5$. A negative configuration energy, in the case of a vacancy, means that the relaxation energy is larger than twice the magnitude of the binding energy per atom $E^a(\text{PC})$ in a perfect crystal. As shown in Fig. 4, compression increases the crystal energy and there is a compression level at which the atom bonding is so weak that removing an atom actually lowers the crystal energy by affording neighboring atoms the freedom to move to positions at which they are more tightly bound than they are in their perfect crystal positions. This occurs at $\eta = 1.27$ and $\eta = 1.46$, respectively, for uniaxial and isotropic compression.

The SCV relaxation energy is shown in Fig. 9. The relaxation energy increases monotonically with isotropic compression. In contrast, the relaxation energy rises to a maximum at about $\eta = 1.36$ and then falls rapidly for $\eta > 1.36$ when the crystal is compressed uniaxially. The compression regime associated with the relaxation energy peak during uniaxial compression corresponds closely to that for a negative vacancy formation energy for that type of compression. In this context it is interesting to note that the atom displacement magnitudes also reach a peak within the compression regime 1.30-1.375. This feature is described by Figs. 25-35 in Sec. V.

Figure 10 allows one to compare the variations in the SCV configuration and relaxation energies with compression and also gives the perfect crystal binding energy per atom $E^a(\text{PC})$ as a function of compression. Note that the relaxation energy exceeds the configuration energy for $\eta > 1.24$. The configuration energy vanishes at $\eta = 1.27$ and the $E^r(\text{SCV})$ and $E^a(\text{PC})$ curves show that $E^r(\text{SCV}) = -2E^a(\text{PC})$ at $\eta = 1.27$.

Figure 11 describes $E^C(\text{SCV})$, $E^r(\text{SCV})$, and $E^a(\text{PC})$ as functions of isotropic compression. Because the isotropically compressed crystal is more stable than the uniaxially compressed crystal (see Fig. 4), the relaxation energy for the isotropic case is small compared with that for the uniaxial case. A relaxation energy peak, such as that seen in Fig. 10 for uniaxial compression, does not occur for $1.0 \leq \eta \leq 1.5$ in the isotropic compression calculations.

Fig. 8.
SCV configuration energy vs compression.

Fig. 9.
SCV relaxation energy vs compression.

Fig. 10.
Composite plot of E^c (SCV), E^r (SCV),
and E^a (PC) for uniaxial compression.

Fig. 11.

Composite plot of $E^c(\text{SCV})$, $E^r(\text{SCV})$, and $E^a(\text{PC})$ for isotropic compression.

Tables VII and VIII contain the numerical data upon which the discussion of the SCV was based. One aspect of these data which has not been discussed is the relaxation intensity $I_r(\text{SCV})$. Table VII shows that the uniaxial compression regime for which $I_r(\text{SCV})$ exceeds unity also corresponds to that in which $E^r(\text{SCV})$ exceeds $-2E^a(\text{PC})$ and in which $E^a(\text{PC})$ is negative. In the case of isotropic compression, $I_r(\text{SCV})$ exceeds unity only for $1.47 \leq \eta \leq 1.5$, as is shown in Table IX. The $E^c(\text{SCV})_{\text{ur}}$ and $E^r(\text{SCV})$ values used to prepare Table IX were read from plots of the data given in Table VIII.

TABLE VII

Uniaxial Compression: Site-centered vacancy energies expressed in eV. $E^x(V)$ is the crystal energy, $E^x(V)_{\text{ur}}$ is the unrelaxed crystal energy, and $E^r(V)$ is the vacancy relaxation energy. $E^c(V)$ and $E^c(V)_{\text{ur}}$ are the vacancy configuration energy and unrelaxed configuration energy, respectively.

η	$E^x(V)_{\text{ur}}$	$E^x(V)$	$E^r(V)$
1.0	-34.352081	-34.352081	0.0
1.10	-34.844768	-34.848702	0.003934
1.20	-31.866812	-31.888546	0.021734
1.25	-28.653494	-28.725545	0.072051
1.30	-24.396812	-24.590117	0.193305
1.33	-20.957933	-21.297143	0.339210
1.375	-15.952484	-16.383774	0.431290
1.414	-10.482539	-10.694824	0.212285
1.50	4.188728	4.173256	0.015472

η	$E^c(V)_{\text{ur}}$	$E^c(V)$	$E^r(V)/E^c(V)_{\text{ur}}$
1.0	0.137987	0.137987	0.0
1.10	0.139954	0.136020	0.0281
1.20	0.127990	0.106256	0.1698
1.25	0.115076	0.043025	0.6261
1.30	0.097968	-0.095337	1.9731
1.33	0.084168	-0.255042	4.0302
1.375	0.064044	-0.367246	6.7343
1.414	0.042090	-0.170195	5.0436
1.50	-0.016827	-0.032299	0.0195

TABLE VIII

Isotropic Compression: Site-centered vacancy energies expressed in eV. $E^x(V)$ is the crystal energy, $E^x(V)_{\text{ur}}$ is the unrelaxed crystal energy, and $E^r(V)$ is the vacancy relaxation energy. $E^c(V)$ and $E^c(V)_{\text{ur}}$ are the vacancy configuration energy and unrelaxed configuration energy, respectively.

η	$E^x(V)_{\text{ur}}$	$E^x(V)$	$E^r(V)$
1.0	-34.352081	-34.352081	0.0
1.15	-34.816905	-34.819528	0.002623
1.20	-33.256892	-33.261809	0.004917
1.25	-30.822105	-30.830005	0.007900
1.30	-27.411318	-27.422759	0.011441
1.375	-20.233915	-20.252108	0.018193
1.50	-1.842477	-1.876274	0.033797

η	$E^c(V)_{\text{ur}}$	$E^c(V)$	$E^r(V)/E^c(V)_{\text{ur}}$
1.0	0.137987	0.137987	0.0
1.15	0.139626	0.137003	0.0188
1.20	0.133726	0.128809	0.0368
1.25	0.123828	0.115928	0.0638
1.30	0.110128	0.098687	0.1039
1.375	0.081252	0.063059	0.2239
1.50	0.007401	-0.026396	4.5665

TABLE IX

$I_r(\text{SCV})$ for isotropic compression $1.46 \leq \eta \leq 1.50$.

η	$I_r(\text{SCV})$	η	$I_r(\text{SCV})$
1.46	0.80	1.49	2.46
1.47	1.07	1.50	4.57
1.48	1.48

Fig. 12.

SV-IP configuration energy vs compression.

Fig. 13.

SV-OP configuration energy vs compression.

2. Split Vacancy. As indicated in Fig. 5, there are two types of SV in a tetragonal crystal; one is the SV-IP described in Fig. 5b and the other is the SV-OP described in Fig. 5d. The SV-IP axis lies in a basal plane, whereas the SV-OP axis runs from one basal plane to another. The SV-IP and SV-OP configuration energies are plotted versus uniaxial

compression in Figs. 12 and 13, respectively. Each of these figures also shows the SV configuration energy for isotropic compression. These and other figures in this section are based on the numerical data listed in Tables X-XIII. As shown in Fig. 14 and Table XII, the relaxed SV-IP and SV-OP have nearly the same

TABLE X

Uniaxial Compression: In-plane mode split-vacancy energies expressed in eV. $E^X(V)$ is the crystal energy, $E^X(V)_{ur}$ is the unrelaxed crystal energy, and $E^r(V)$ is the vacancy relaxation energy. $E^c(V)$ and $E^c(V)_{ur}$ are the vacancy configuration energy and unrelaxed configuration energy, respectively.

η	$E^X(V)_{ur}$	$E^X(V)$	$E^r(V)$
1.0	-34.262591	-34.313054	0.050463
1.10	-34.619240	-34.757901	0.138661
1.20	-31.384385	-31.707631	0.323246
1.25	-27.982088	-28.593145	0.611057
1.30	-23.488438	-24.564352	1.075914
1.33	-19.862219	-21.247055	1.384836
1.375	-14.590136	-16.336243	1.746107
1.50	6.616828	3.003331	3.613497

η	$E^c(V)_{ur}$	$E^c(V)$	$E^r(V)/E^c(V)_{ur}$
1.0	0.227477	0.177014	0.2218
1.10	0.365482	0.226821	0.3794
1.20	0.610417	0.287171	0.5295
1.25	0.786482	0.175425	0.7769
1.30	1.006342	-0.069572	1.0691
1.33	1.179882	-0.204954	1.1737
1.375	1.426392	-0.319715	1.2241
1.50	2.411271	-1.202224	1.4986

TABLE XI

Uniaxial Compression: Out-of-plane mode split-vacancy energies expressed in eV. $E^X(V)$ is the crystal energy, $E^X(V)_{ur}$ is the unrelaxed crystal energy, and $E^r(V)$ is the vacancy relaxation energy. $E^c(V)$ and $E^c(V)_{ur}$ are the vacancy configuration energy and unrelaxed configuration energy, respectively.

η	$E^X(V)_{ur}$	$E^X(V)$	$E^r(V)$
1.0	-34.262591	-34.313054	0.050363
1.10	-34.745444	-34.802136	0.056692
1.20	-31.762538	-31.837834	0.075296
1.25	-28.550203	-28.691420	0.141218
1.30	-24.291882	-24.607917	0.316035
1.33	-20.850938	-21.334545	0.483607
1.375	-15.840835	-16.454907	0.614073
1.414	-10.362695	-10.626707	0.264012
1.50	4.357579	2.990832	1.366747

η	$E^c(V)_{ur}$	$E^c(V)$	$E^r(V)/E^c(V)_{ur}$
1.0	0.227477	0.177014	0.2218
1.10	0.239278	0.182586	0.2369
1.20	0.232264	0.156968	0.3242
1.25	0.218367	0.077165	0.6467
1.30	0.202898	-0.113137	1.5576
1.33	0.191163	-0.292444	2.5298
1.375	0.175693	-0.438379	3.4951
1.414	0.161934	-0.102078	1.6304
1.50	0.152024	-1.214723	8.9903

TABLE XII

Uniaxial Compression: The difference $E^c_{ip}(V) - E^c_{op}(V)$ between the in-plane and the out-of-plane mode split-vacancy configuration energies; (a) unrelaxed, (b) relaxed. All energies are expressed in eV.

η	(a) Unrelaxed	(b) Relaxed
1.0	0.0	---
1.10	0.126204	0.044235
1.20	0.378153	0.130203
1.25	0.568115	0.098260
1.30	0.803444	0.043565
1.33	0.988719	0.087490
1.375	1.264458	0.118664
1.50	2.259249	0.012499

TABLE XIII

Isotropic Compression: Split-vacancy energies expressed in eV. $E^X(V)$ is the crystal energy, $E^X(V)_{ur}$ is the unrelaxed crystal energy, and $E^r(V)$ is the vacancy relaxation energy. $E^c(V)$ and $E^c(V)_{ur}$ are the vacancy configuration energy and unrelaxed configuration energy, respectively.

η	$E^X(V)_{ur}$	$E^X(V)$	$E^r(V)$
1.0	-34.262591	-34.313054	0.050463
1.15	-34.648087	-34.736593	0.088506
1.20	-33.053327	-33.171336	0.118009
1.25	-30.582121	-30.722715	0.140594
1.30	-27.126753	-27.295178	0.168425
1.375	-19.871463	-20.088960	0.217497
1.50	-1.321043	-1.684286	0.362343

η	$E^c(V)_{ur}$	$E^c(V)$	$E^r(V)/E^c(V)_{ur}$
1.0	0.227477	0.177014	0.2218
1.15	0.308444	0.219938	0.2869
1.20	0.337291	0.219282	0.3499
1.25	0.363812	0.223218	0.3864
1.30	0.394693	0.226268	0.4267
1.375	0.443704	0.226207	0.4902
1.50	0.527935	0.165592	0.6863

configuration energy. However, the difference in the unrelaxed configuration energies for the SV-IP and SV-OP increases monotonically with uniaxial compression. The SV-IP and SV-OP configuration energies are negative for $\eta > 1.285$ and $\eta > 1.276$, respectively. A sharp peak occurs in the SV-IP configuration energy at about $\eta = 1.21$. In contrast, the SV-OP configuration energy rises slightly to a flat peak at $\eta \approx 1.10$ and thereafter decreases rapidly for $\eta > 1.2$.

Tables X and XI show that the SV configuration energy continues to fall with increasing uniaxial compression up to $\eta = 1.5$. Recall that $E^c(\text{SCV})$ exhibited a minimum at $\eta = 1.365$, as is shown in Fig. 10.

Figure 15 shows that the SV-IP relaxation energy exceeds that for the SV-OP. The datum point at $\eta = \sqrt{2}$ (bcc structure) for the SV-OP stands apart from the other data points. This feature suggests that additional runs are needed to better define the SV relaxation energy for $1.375 \leq \eta \leq 1.5$.

The SV and SCV configuration energies are plotted in Fig. 16 for isotropic compression. $E^c(\text{SV})$ rises to a plateau at $\eta = 1.15$ and then once more rises slightly to a broad maximum at $\eta = 1.33$, and it is positive for all compressions considered. In contrast,

Fig. 14.
Configuration energy difference for SV-IP and SV-OP in the case of uniaxial compression.

Fig. 15.
Split vacancy relaxation energy for uniaxial compression.

Fig. 16.

SCV and SV configuration energies for isotropic compression.

$E^C(\text{SCV})$ decreases with increasing isotropic compression and becomes negative at $\eta = 1.47$.

A summary of the relaxation intensity results for vacancies is given in Fig. 17. I_r rises to a maximum at $\eta = 1.375$ for an SCV during uniaxial compression. In all other cases, I_r increases monotonically with compression up to $\eta = 1.5$.

C. Vacancy Formation Energy

The vacancy formation energy recipe defined in Sec. IV.A is

$$E^f(V) = E^C(V) + E^{\text{cl}}(\text{PC}) \quad . \quad (12)$$

In the case of an SCV, this can be written as

$$E^f(\text{SCV}) = -[E^a(\text{PC}) + E^f(\text{SCV})] \quad , \quad (14)$$

and in the case of an SV, it is

Fig. 17.

Composite plot of SCV and SV relaxation intensities.

$$E^f(\text{SV}) = E^c(\text{SV})_{\text{ur}} - E^r(\text{SV}) + E^a(\text{PC}) \quad (15)$$

$E^f(\text{SCV})$ and $E^f(\text{SV})$ were computed for uniaxial and isotropic compression using the configuration and relaxation energy data given in Tables VII, VIII, X, and XI, together with the $E^a(\text{PC})$ data given in Tables IV and V. The formation energy results are listed in Tables XIV and XV. The positive formation energies are plotted in Figs. 18 and 19. As indicated by Eq. (14), $E^f(\text{SCV})$ is dominated

TABLE XIV

Uniaxial Compression: Vacancy formation energies expressed in eV.

r_i	$E^f(\text{SCV})$	$E^f(\text{SV-IP})$	$E^f(\text{SV-OP})$
1.0	0.0690	0.1080	0.1080
1.10	0.0660	0.1568	0.1123
1.20	0.0423	0.2232	0.0930
1.25	-0.0145	0.1179	0.0196
1.30	-0.1443	-0.1186	-0.1621
1.33	-0.2971	-0.2470	-0.3345
1.375	-0.3993	-0.3517	-0.4704
1.414	-0.1912	---	-0.1231
1.50	-0.0239	-1.1938	-1.2063

TABLE XV

Isotropic Compression: Vacancy formation energies expressed in eV.

η	$E^a(\text{PC})$	$E^f(\text{SCV})$	$E^f(\text{SV})$
1.0	-0.068980	0.069007	0.108034
1.10	-0.069437	---	---
1.15	-0.069913	0.067090	0.150025
1.20	-0.066781	0.062028	0.152501
1.25	-0.061892	0.054036	0.161326
1.30	-0.055043	0.043644	0.171225
1.375	-0.040630	0.022429	0.185577
1.50	-0.003700	-0.030096	0.161892

Fig. 18.

SCV, SV-OP, and SV-IP formation energies for uniaxial compression.

Fig. 19.

SCV and SV formation energies for isotropic compression.

by $-E^a(PC)$ for compression up to 1.2 because $E^r(SCV)$ is small for both uniaxial and isotropic compression below 1.2. Consequently, $E^f(SCV)$ does not increase with compression because $-E^a(PC)$ does not increase with compression. The role of $E^r(V)$ always is to reduce the formation energy. The out-of-plane SV formation energy behavior for uniaxial compression is similar to that for an SCV but is larger than the SCV formation energy at a given compression.

Both the uniaxial compression in-plane SV and the isotropic compression SV exhibit a larger unrelaxed configuration energy than do either the SCV or the in-plane SV, and these unrelaxed configuration energies increase with compression. Thus, in accordance with Eq. (15), the isotropic compression SV and the uniaxial compression in-plane SV exhibit a formation energy which increases with compression up to $\eta = 1.21$ for uniaxial compression and $\eta = 1.4$ for isotropic compression.

D. Vacancy Migration Energy

In this discussion, it is assumed that (1) the stable vacancy form in an fcc Lennard-Jones crystal is either the SCV, SV-OP, or SV-IP configuration; (2) if the SCV is the stable form, then an SV is the vacancy migration saddle-point configuration; and (3) if an SV is the stable form, then the vacancy migration saddle-point configuration is either the SCV or the other SV. Assumption (1) virtually is dictated by crystal symmetry. The vacancy migration examples given by Beeler and Beeler (1979) for fcc, bcc, and hcp crystals show that assumptions (2) and (3) should lead to very good estimates of the vacancy migration energy even if the actual saddle-point configurations turned out to be slightly different from those assumed.

Three- and four-point Lagrangian interpolation, applied to the vacancy configuration data in Tables VII, VIII, X, XI, and XIII, was used to prepare more "refined" plots of vacancy configuration energy versus compression than one can make using the direct data given in the tables cited. This was done in order to estimate what particular vacancy form was the stable vacancy form and what particular vacancy form was the vacancy migration saddle point as a function of compression. Table XVI gives the interpolated configuration energy results for uniaxial compression $1.16 \leq \eta \leq 1.30$. These results are the basis for Fig. 20. Table XVII gives the interpolation results for uniaxial compression $1.30 \leq \eta \leq 1.50$. These results are the basis for Fig. 21. Taken together, Figs. 20 and 21 show the following relative ordering among $E^c(SCV)$, $E^c(SV-OP)$, and $E^c(SV-IP)$.

TABLE XVI

Uniaxial Compression: Interpolated
vacancy configuration energies expressed
in eV for $1.16 \leq \eta \leq 1.30$.

η	$E^c(\text{SV-OP})$	$E^c(\text{SV-IP})$	$E^c(\text{SCV})$
1.16	0.174	---	0.127
1.18	0.168	---	0.119
1.20	0.157	---	0.106
1.22	0.132	---	0.087
1.24	0.099	---	0.061
1.26	0.053	0.148	0.026
1.28	-0.015	0.069	-0.022
1.30	-0.113	-0.071	-0.095

Fig. 20.

SCV, SV-OP, and SV-IP configuration energies in the compression region in which they become negative for uniaxial compression.

TABLE XVII

Uniaxial Compression: Interpolated
vacancy configuration energies expressed
in eV for $1.30 \leq \eta \leq 1.50$.

η	$E^c(\text{SV-OP})$	$E^c(\text{SV-IP})$	$E^c(\text{SCV})$
1.3	-0.113	-0.071	-0.095
1.32	-0.220	-0.155	-0.180
1.34	-0.335	-0.225	-0.305
1.36	-0.402	-0.275	-0.375
1.38	-0.460	-0.340	-0.350
1.40	-0.530	-0.430	-0.230
1.42	-0.625	-0.535	-0.150
1.44	-0.740	-0.665	-0.100
1.46	-0.875	-0.815	-0.070
1.48	-1.07	-0.995	-0.045
1.50	-1.21	-1.20	-0.030

Fig. 21.

Crossing of the SCV and SV-IP configuration energies at $\eta = 1.382$.

$$\begin{aligned}
E^C(\text{SCV}) &< E^C(\text{SV-OP}) < E^C(\text{SV-IP}) & 1.0 \leq \eta < 1.286 \\
E^C(\text{SCV}) &= E^C(\text{SV-OP}) < E^C(\text{SV-IP}) & \eta = 1.286 \\
E^C(\text{SV-OP}) &< E^C(\text{SCV}) < E^C(\text{SV-IP}) & 1.286 < \eta < 1.382 \\
E^C(\text{SCV}) &= E^C(\text{SV-IP}) & \eta = 1.382 \\
E^C(\text{SV-OP}) &< E^C(\text{SV-IP}) < E^C(\text{SCV}) & 1.382 < \eta \leq 1.50
\end{aligned}$$

These relative ordering relations imply the stable vacancy and vacancy migration saddle-point statements given in Table XVIII for uniaxial compression. Table XIX summarizes the vacancy configuration energy data and derived migration energy results for uniaxial compression.

In the case of isotropic compression, the migration process is straightforward. $E^C(\text{SV}) > E^C(\text{SCV})$ for all compression levels concerned and so the SCV is the stable configuration and the SV is the vacancy migration saddle point. Table XX summarizes the vacancy configuration energy data and the derived vacancy migration energy for isotropic compression.

TABLE XVIII

Stable vacancy and vacancy migration saddle point configurations as a function of compression.

Compression Mode	Compression Range	Stable Vacancy	Vacancy Migration Saddle Point
Isotropic	0.97 - 1.5	SCV	SV
Uniaxial	1.0 - 1.286	SCV	SV-OP
Uniaxial	1.286 - 1.382	SV-OP	SCV
Uniaxial	1.382 - 1.50	SV-OP	SV-IP

TABLE XX

Isotropic Compression: Vacancy configuration energies and migration energy expressed in eV as functions of compression.

η	$E^C(\text{SCV})$	$E^C(\text{SV})$	E^m
1.0	0.1380	0.1770	0.0390
1.15	0.1370	0.2199	0.0829
1.20	0.1288	0.2193	0.0905
1.25	0.1159	0.2232	0.1073
1.30	0.0987	0.2263	0.1276
1.375	0.0631	0.2262	0.1631
1.50	-0.0264	0.1656	0.1920

TABLE XIX

Uniaxial Compression: Vacancy configuration energies and migration energy expressed in eV as functions of compression.

η	$E^C(\text{SCV})$	$E^C(\text{SV-OP})$	$E^C(\text{SV-IP})$	E^m
1.0	0.1380 ^{sc}	0.1770 ^{sp}	0.1770	0.0390
1.1	0.1360 ^{sc}	0.1826 ^{sp}	0.2268	0.0466
1.2	0.1062 ^{sc}	0.1570 ^{sp}	0.2872	0.0508
1.25	0.0430 ^{sc}	0.0772 ^{sp}	0.1754	0.0342
1.286	-0.0400	-0.0400	0.0350	0.0
1.30	-0.0953 ^{sp}	-0.1131 ^{sc}	-0.0696	0.0178
1.33	-0.2550 ^{sp}	-0.2924 ^{sc}	-0.2050	0.0374
1.35	-0.36 ^{sp}	-0.38 ^{sc}	-0.25	0.02
1.375	-0.3672 ^{sp}	-0.4384 ^{sc}	-0.3197	0.0712
1.382	-0.345	-0.465	-0.345	0.120
1.40	-0.23	-0.53 ^{sc}	-0.43 ^{sp}	0.10
1.45	-0.08	-0.80 ^{sc}	-0.74 ^{sp}	0.06
1.50	-0.0322	-1.2147 ^{sc}	-1.2022 ^{sp}	0.0125

sc = stable configuration.
sp = saddle point.

The vacancy migration energy is plotted in Fig. 22 for both uniaxial and isotropic compression. The migration energy for isotropic compression exceeds that for uniaxial compression for all compressions and exhibits a nearly linear rise with compression. In the case of uniaxial compression, there is a window region, $1.25 < \eta < 1.35$, within which the vacancy migration energy is less than 0.039 eV, the migration energy at $\eta = 1.0$. Within the window region the migration energy drops to zero at $\eta = 1.286$. A peak of 0.12 eV occurs at $\eta = 1.38$, after which the migration energy falls almost linearly to 0.0125 eV at $\eta = 1.5$. This peak occurs at a compression near that ($\eta = \sqrt{2}$) which gives a bcc structure.

Fig. 22.
Vacancy migration energy vs compression.

V. VACANCY DISPLACEMENT FIELD IN A COMPRESSED CRYSTAL

This section deals with the displacement field of a vacancy in a compressed crystal. In Sec. IV, we showed that the SCV was a stable vacancy configuration in each of the isotropic compression runs for $0.94 \leq \eta \leq 1.5$. In the case of uniaxial compression, the SCV was the stable vacancy configuration for $\eta < 1.29$, but for $1.29 < \eta < 1.5$, the SV-OP was the stable configuration. The vacancy displacement field pattern for $\eta < 1.29$ is qualitatively different from that for $1.29 < \eta$ and the nature of this difference illustrates why uniaxial compression changes the form of the stable vacancy, whereas isotropic compression does not. The discussion deals first with the SCV and then the SV-OP.

Vacancy displacement fields provide useful insight concerning the stability of a crystal subjected to uniaxial compression. Because all real crystals contain vacancy defects and edge dislocation line segments, the observations given here on the effect of uniaxial compression on a vacancy displacement field are of fundamental as well as technological interest in the interpretation of shock process data. Edge dislocation line segments are included in this context because the core of an edge dislocation behaves, in part, as a line of vacancies. In

particular, extended shear displacements observed in a uniaxially compressed crystal containing a line of vacancies should also occur on the tension stress side of an edge dislocation in a uniaxially compressed crystal. In contrast, vacancy displacement field results for isotropic compression appear to shed little light on shock processes in crystals containing tension stress field defects.

A. SCV Displacement Field: Isotropic Compression

The SCV displacement field results for isotropic compression $1.0 < \eta \leq 1.5$ are qualitatively the same as those for $\eta = 1$. This is true because isotropic compression does not alter the crystal symmetry. Tables XXI-XXVI describe the SCV displacement field for the first five neighbor shells in the case of isotropic compression.

No atom relaxation occurred about the vacant site for $\eta = 1.0$. This was an unexpected result. Because the first simulation was done by creating a vacancy at site 225 in a perfect crystal, it was speculated that perhaps lock-in effects due to perfect crystal symmetry precluded relaxation. Hence, a second simulation was done, in which random initial atom displacements were assigned to break up any possible symmetry lock-in effects. The average displacement was about 0.01 hlc (see Appendix B). However, the result again was no atom relaxation about a vacancy at $\eta = 1.0$. In this regard, Fig. 4b shows that the crystal is subjected to a negative pressure at $\eta = 1.0$. We conclude that the null relaxation result for $\eta = 1.0$ is a particular consequence of this negative pressure because Table VIII shows that relaxation about an SCV did occur at all other compression levels.

As the compression was increased to 1.5, significant relaxation occurred only within the first four neighbor shells. At each compression level cited in Tables XXII-XXVI, first-, third-, and fourth-neighbor atoms relaxed inward and second-neighbor atoms relaxed outward from the vacancy. Table XXVI and Fig. 23 express the first-neighbor atom relaxation as a fraction of the interatomic distance at the compression cited. There first-neighbor relaxations ranged from 1.0% to 1.8% of the interatomic distance over the compression interval $1.15 \leq \eta \leq 1.50$.

Figure 24 is a map of the site-centered vacancy displacement field in the $y = 4.5$ plane for a vacancy at site 225 and $\eta = 1.5$. Sites 173, 175, 273, and 275 are first-neighbor sites. Sites 123, 127, 323, and 327 are fourth-neighbor sites. The displacement magnitudes in Fig. 24 are magnified by a factor of five (5X). Second-neighbor atom displacements at sites 125, 223, 227, and 325 are too small to be resolved in Fig. 24 at 5X magnification. There are no third-neighbor

TABLE XXI

Vacancy displacement field for isotropic compression $\eta = 1.15$. Site coordinates are expressed in hlc. Atom displacement components are expressed in basal plane hlc.

Site No.	Shell No., n	X	Y	Z	DX	DY	DZ	DR
226	1	5.5	5.5	4.5	-0.0100	-0.0100	0.0	0.0141
227	2	6.5	4.5	4.5	0.0033	0.0	0.0	0.0033
278	3	6.5	5.5	5.5	-0.0022	-0.0017	-0.0017	0.0032
237	4	6.5	6.5	4.5	-0.0031	-0.0031	0.0	0.0044
228	5	7.5	5.5	4.5	0.0004	0.0	0.0	0.0004

TABLE XXII

Vacancy displacement field for isotropic compression $\eta = 1.20$. Site coordinates are expressed in hlc. Atom displacement components are expressed in basal plane hlc.

Site No.	Shell No., n	X	Y	Z	DX	DY	DZ	DR
226	1	5.5	5.5	4.5	-0.0120	-0.0120	0.0	0.0170
227	2	6.5	4.5	4.5	0.0030	0.0	0.0	0.0030
278	3	6.5	5.5	5.5	-0.0028	-0.0022	-0.0028	0.0045
237	4	6.5	6.5	4.5	-0.0037	-0.0037	0.0	0.0052
228	5	7.5	5.5	4.5	0.0005	0.0	0.0	0.0005

TABLE XXIII

Vacancy displacement field for isotropic compression $\eta = 1.25$. Site coordinates are expressed in hlc. Atom displacement components are expressed in basal plane hlc.

Site No.	Shell No., n	X	Y	Z	DX	DY	DZ	DR
226	1	5.5	5.5	4.5	-0.0136	-0.0136	0.0	0.0192
227	2	6.5	4.5	4.5	0.0030	0.0	0.0	0.0030
278	3	6.5	5.5	5.5	-0.0034	-0.0024	-0.0024	0.0048
237	4	6.5	6.5	4.5	-0.0043	-0.0043	0.0	0.0061
228	5	7.5	5.5	4.5	0.0004	-0.0002	0.0	0.0004

TABLE XXIV

Vacancy displacement field for isotropic compression $\eta = 1.30$. Site coordinates are expressed in hlc. Atom displacement components are expressed in basal plane hlc.

Site No.	Shell No.,n	X	Y	Z	DX	DY	DZ	DR
226	1	5.5	5.5	4.5	-0.0147	-0.0147	0.0	0.0208
227	2	6.5	4.5	4.5	0.0026	0.0	0.0	0.0026
278	3	6.5	5.5	5.5	-0.0039	-0.0028	-0.0028	0.0056
237	4	6.5	6.5	4.5	-0.0048	-0.0048	0.0	0.0068
228	5	7.5	5.5	4.5	0.0003	-0.0002	0.0	0.0004

TABLE XXV

Vacancy displacement field for isotropic compression $\eta = 1.375$. Site coordinates are expressed in hlc. Atom displacement components are expressed in basal plane hlc.

Site No.	Shell No.,n	X	Y	Z	DX	DY	DZ	DR
226	1	5.5	5.5	4.5	-0.0162	-0.0162	0.0	0.0229
227	2	6.5	4.5	4.5	0.0024	0.0	0.0	0.0024
278	3	6.5	5.5	5.5	-0.0044	-0.0032	-0.0032	0.0063
237	4	6.5	6.5	4.5	-0.0054	-0.0054	0.0	0.0076
228	5	7.5	5.5	4.5	0.0002	0.0002	0.0	0.0002

TABLE XXVI

Vacancy displacement field for isotropic compression $\eta = 1.50$. Site coordinates are expressed in hlc. Atom displacement components are expressed in basal plane hlc.

Site No.	Shell No.,n	X	Y	Z	DX	DY	DZ	DR
226	1	5.5	5.5	4.5	-0.0179	-0.0179	0.0	0.0252
227	2	6.5	4.5	4.5	0.0022	0.0	0.0	0.0022
278	3	6.5	5.5	5.5	-0.0049	-0.0036	-0.0036	0.0062
237	4	6.5	6.5	4.5	-0.0059	-0.0059	0.0	0.0083
228	5	7.5	5.5	4.5	0.0002	-0.0004	0.0	0.0004

atom sites in the $y = 4.5$ plane. The coordinates in Fig. 24 are expressed in half-lattice-constant (hlc) units at a compression of 1.5.

Fig. 23.
First-neighbor radial displacement $DR(1)$ expressed as a fraction of the basal plane interatomic distance d_1 for an SCV and isotropic compression.

Fig. 24.
SCV displacement field map for isotropic compression equal to 1.50. The $y = 4.5$ plane shown here passes through the vacancy at site 225. The displacement component DY is zero for all atoms in the $y = 4.5$ plane. The radius of each circle used to denote site positions is equal to 1% of the basal plane interatomic distance at a magnification $\times 5X$. The length of the radial line drawn from the center of a circle is the radial displacement vector at magnification $\times 5X$.

B. Site-Centered Vacancy Displacement Field: Uniaxial Compression

Figures 25-35 are plots of atom relaxation about a site-centered vacancy at site 225 versus uniaxial compression along [001], for each of the first ten neighbor shells. The neighbor shell designation cited pertains to the location of the atom noted in an fcc crystal when $\eta = 1.0$. These figures show that displacement magnitudes for the first-, second-, and third-neighbor shells tend to increase as compression increases up to $\eta = 1.3$ and then tend to decrease as compression increases from 1.3 to 1.5. Displacement magnitudes in the fourth- and tenth-neighbor shells increase with increasing compression up to $\eta = 1.375$, and then

Fig. 25.

Radial displacement in basal plane half-lattice constants for in-plane and out-of-plane first neighbors of an SCV vs uniaxial compression.

Fig. 26.

Radial displacement for second neighbors of an SCV vs uniaxial compression.

Fig. 27.

Radial displacement for third neighbors of an SCV vs uniaxial compression.

Fig. 28.

Radial displacement for fourth neighbors of an SCV vs uniaxial compression.

Fig. 29.

Radial displacement for fifth neighbors of an SCV vs uniaxial compression.

Fig. 30.

Radial displacement for sixth neighbors of an SCV vs uniaxial compression.

Fig. 31.

Radial displacement for seventh neighbors of an SCV vs uniaxial compression.

Fig. 32.

Radial displacement for eighth neighbors of an SCV vs uniaxial compression.

decrease as compression increases from 1.375 to 1.50. In most instances, the displacement magnitudes for the out-of-plane subshells are greater than those for the in-plane subshells. A description of in-plane and out-of-plane neighbor subshells is given in Appendix C.

In short, out-of-plane displacements about the vacancy increase with uniaxial compression up to a certain compression level as the result of augmented displacement components parallel to the uniaxial compression stress axis. However, this effect eventually is thwarted when the increase in atom number density, due to increasing compression, begins to restrict the range of atom movement. In

Fig. 33.

Radial displacement for [330] and [303] ninth neighbors of an SCV vs uniaxial compression.

Fig. 34.

Radial displacement for [411] and [114] ninth neighbors of an SCV vs uniaxial compression.

Fig. 35.

Radial displacement for [420] and [204] tenth neighbors of an SCV vs uniaxial compression.

other words, increasing compression leads to a crowding effect which tends to reduce individual atom displacement magnitudes even though the repulsive force atom pair interaction increases monotonically with compression. The attenuating effect of crowding on first-neighbor atom relaxation about a vacancy, in the case of isotropic compression, is illustrated in Fig. 23. This figure suggests a saturation effect for isotropic compression.

Displacement field maps are given in Figs. 36-42 for uniaxial compression.

Each of these maps describes the displacement of atoms in the $y = 4.5$ plane through a site-centered vacancy at site 225. At $\eta = 1.10$ (Fig. 36), the displacement map resembles that for isotropic compression $\eta = 1.50$ (see Fig. 24) in that only the relaxation of first-neighbor atoms is significant. As compression increases, one notices that the number of atom sites at which the atom displacement exceeds 1% of the interatomic distance (measured at $\eta = 1.0$) also increases. Atom displacements are listed in Tables XXVII-XXXIII.

Fig. 36.

Displacement field map for the $y = 4.5$ plane through an SCV for uniaxial compression equal to 1.10. The radius of each circle used to denote the position of an atom site is equal to 1% of the basal plane interatomic distance at a magnification of 5X. The radial line marked for a site is the radial atom displacement at that site at magnification 5X. This notation is used in each succeeding displacement field map.

Fig. 37.

Displacement field map for the $y = 4.5$ plane through an SCV for uniaxial compression equal to 1.20.

Fig. 38.

Displacement field map for the $y = 4.5$ plane through an SCV for uniaxial compression equal to 1.25.

Fig. 39.

Displacement field map for the $y = 4.5$ plane through an SCV for uniaxial compression equal to 1.30.

Fig. 40.
Displacement field map for the $y = 4.5$ plane through an SCV for uniaxial compression equal to 1.375.

Fig. 41.
Displacement field map for the $y = 4.5$ plane through an SCV for uniaxial compression equal to 1.414.

Fig. 42.
Displacement field map for the $y = 4.5$ plane through an SCV for uniaxial compression equal to 1.50.

Fig. 43.
First-neighbor displacement vector angle for an SCV.

Figure 43 and Table XXXIV describe the variation of the angle θ between the out-of-plane first-neighbor displacement vector for the atom at site 173 and the line from site 173 to the vacant site at site 225, as η increases from 1.0 to 1.5. θ is positive and increases with increasing η up to $\eta = 1.275$. This means that the displacement vector deviates progressively from the site-to-site line direction toward the z -axis. θ then decreases from a maximum of 22° to zero as η increases from 1.275 to 1.425. Thereafter, θ becomes progressively more negative

TABLE XXVII

Uniaxial Compression $\eta = 1.10$: 3CV displacement field (DX, DY, DZ) in the $y = 4.5$ plane through the vacancy at site 225. $DY = 0$ for all sites in the $y = 4.5$ plane. DX, DY, and DR are expressed in h/c (xy).

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0016	0.0	0.0016	221	-0.0006	0.0	0.0006
473	0.0003	0.0	0.0003	223	-0.0069	0.0	0.0069
475	-0.0003	0.0	0.0003	225	0.0	0.0	0.0
477	-0.0017	0.0	0.0017	227	0.0068	0.0	0.0068
479	0.0	0.0	0.0	229	0.0007	0.0	0.0007
421	0.0022	-0.0009	0.0024	171	-0.0022	-0.0014	0.0026
423	0.0013	-0.0009	0.0016	173	0.0191	0.0283	0.0341
425	0.0	0.0	0.0	175	-0.0189	0.0283	0.0340
427	-0.0013	-0.0009	0.0016	177	0.0023	-0.0014	0.0027
429	-0.0023	-0.0009	0.0025	179	0.0	-0.0005	0.0005
371	0.0043	-0.0036	0.0056	121	-0.0008	-0.0012	0.0014
373	0.0010	-0.0011	0.0015	123	0.0092	0.0092	0.0130
375	-0.0011	-0.0011	0.0016	125	0.0	0.0005	0.0005
377	-0.0044	0.0036	0.0057	127	-0.0092	0.0092	0.0130
379	0.0	0.0013	0.0013	129	0.0007	-0.0012	0.0014
321	-0.0008	0.0012	0.0014	71	0.0043	0.0036	0.0056
323	0.0092	-0.0093	0.0131	73	0.0010	0.0011	0.0015
325	0.0	-0.0006	0.0006	75	-0.0011	0.0011	0.0016
327	-0.0092	-0.0093	0.0131	77	-0.0044	0.0036	0.0057
329	0.0067	0.0012	0.0014	79	0.0	-0.0013	0.0013
271	-0.0022	0.0014	0.0026	21	0.0022	0.0008	0.0023
273	0.0188	-0.0282	0.0339	23	0.0013	0.0008	0.0015
275	-0.0189	-0.0282	0.0339	25	0.0	0.0	0.0
277	0.0023	0.0014	0.0027	27	-0.0013	0.0008	0.0015
279	0.0	0.0005	0.0005	29	-0.0023	0.0008	0.0024

as η increases to 1.5. This means that for $\eta > 1.425$, the displacement vector deviates progressively from the site-to-site line toward the x-axis. In a qualitative sense, uniaxial stress first tends to rotate the atom displacement vector away from the close-packed line direction toward the stress axis for $\eta < 1.275$. This effect persists with diminishing strength up to $\eta = 1.425$. Thereafter, an increase in axial stress inhibits displacement along the stress axis and produces a relatively greater displacement component normal to the stress axis.

The behavior described by Table XXXIV and Fig. 43 is critical behavior in that for $1.275 < \eta < 1.425$ the crystal is in a transition region, due to the

TABLE XXVIII

Uniaxial Compression $\eta = 1.20$: SCV displacement field (DX, DY, DZ) in the $y = 4.5$ plane through the vacancy at site 225. $DY = 0$ for all sites in the $y = 4.5$ plane. DX, DY, and DR are expressed in hlc (xy).

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0094	0.0	0.0	221	0.0013	0.0	0.0013
473	-0.0014	0.0	0.0014	223	-0.0151	0.0	0.0151
475	0.0013	0.0	0.0012	225	0.0	0.0	0.0
477	-0.0095	0.0	0.0095	227	0.0151	0.0	0.0151
479	-0.0082	0.0	0.0082	229	-0.0013	0.0	0.0013
421	0.0118	-0.0029	0.0122	171	-0.0043	-0.0098	0.0107
423	0.0057	-0.0056	0.0080	173	0.0474	0.0796	0.0927
425	0.0	0.0050	0.0050	175	-0.0474	0.0796	0.0927
427	-0.0058	-0.0056	0.0080	177	0.0042	-0.0112	0.0119
429	-0.0117	-0.0029	0.0121	179	0.0	-0.0013	0.0013
371	0.0177	-0.0168	0.0245	121	-0.0042	-0.0083	0.0092
373	0.0081	-0.0046	0.0093	123	0.0337	0.0308	0.0456
375	-0.0080	-0.0046	0.0092	125	0.0	0.0144	0.0144
377	-0.0177	-0.0168	0.0245	127	-0.0336	0.0307	0.0456
379	0.0	0.0114	0.0114	129	0.0042	-0.0082	0.0093
321	-0.0042	0.0083	0.0092	71	0.0177	0.0168	0.0245
323	-0.0337	-0.0308	0.0456	73	0.0081	0.0045	0.0093
325	0.0	-0.0144	0.0144	75	-0.0080	0.0045	0.0092
327	-0.0336	-0.0308	0.0456	77	-0.0177	0.0168	0.0245
329	0.0042	0.0083	0.0093	79	0.0	-0.0114	0.0114
271	-0.0043	0.0112	0.0120	21	0.0118	0.0029	0.0122
273	0.0474	-0.0796	0.0927	23	0.0057	0.0056	0.0080
275	-0.0474	-0.0796	0.0927	25	0.0	-0.0050	0.0050
277	0.0042	0.0134	0.0140	27	-0.0058	0.0056	0.0081
279	0.0	0.0013	0.0013	29	-0.0117	0.0029	0.0121

crowding effect, wherein increased uniaxial compression tends to produce a larger transverse atom displacement, away from the vacancy, than an axial displacement toward the vacancy. This effect is the root from which grow extended shear displacement fields about either an SCV or an SV-OP for $\eta > 1.29$. In an attempt to relieve axial crowding, the crystal turns to transverse crowding.

TABLE XXIX

Uniaxial Compression $\eta = 1.25$: SCV displacement field (DX, DY, DZ) in the $y = 4.5$ plane through the vacancy at site 225. $DY = 0$ for all sites in the $y = 4.5$ plane. DX, DY, and DR are expressed in h/c (xy).

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0203	0.0	0.0203	221	0.0092	0.0	0.0092
473	-0.0053	0.0	0.0053	223	-0.0212	0.0	0.0212
475	0.0054	0.0	0.0054	225	0.0	0.0	0.0
477	-0.0204	0.0	0.0204	227	0.0212	0.0	0.0212
479	0.0	0.0	0.0	229	-0.0092	0.0	0.0092
421	0.0234	-0.0022	0.0235	171	-0.0043	-0.0281	0.0285
423	0.0092	-0.0149	0.0175	173	0.0620	0.1058	0.1226
425	0.0	0.0114	0.0114	175	-0.0619	0.1058	0.1226
427	-0.0092	0.0149	0.0175	177	0.0042	-0.0281	0.0284
429	-0.0233	-0.0022	0.0234	179	0.0	0.0050	0.0050
371	0.0274	-0.0326	0.0425	121	-0.0121	-0.0171	0.0210
373	0.0153	-0.0067	0.0167	123	0.0535	0.0445	0.0696
375	-0.0154	-0.0067	0.0168	125	0.0	0.0234	0.0234
377	-0.0273	-0.0326	0.0425	127	-0.0534	0.0445	0.0696
379	0.0	0.0309	0.0309	129	0.0122	-0.0171	0.0210
321	-0.0121	0.0172	0.0210	71	0.0274	0.0326	0.0426
323	0.0535	-0.0445	0.0696	73	0.0153	0.0067	0.0167
325	0.0	-0.0236	0.0236	75	-0.0154	0.0067	0.0168
327	-0.0534	-0.0445	0.0695	77	-0.0273	0.0326	0.0425
329	0.0122	0.0172	0.0210	79	0.0	-0.0310	0.0310
271	-0.0043	0.0282	0.0285	21	0.0234	0.0021	0.0235
273	0.0620	-0.1059	0.1227	23	0.0092	0.0148	0.0174
275	-0.0619	-0.1059	0.1227	25	0.0	-0.0114	0.0114
277	0.0042	0.0282	0.0285	27	-0.0092	0.0148	0.0174
279	0.0	-0.0049	0.0049	29	-0.0233	0.0021	0.0234

TABLE XXX

Uniaxial Compression $\eta = 1.30$: SCV displacement field (DX, DY, DZ) in the $y = 4.5$ plane through the vacancy at site 225. DY = 0 for all sites in the $y = 4.5$ plane. DX, DY, and DR are expressed in h/c (xy).

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0387	0.0	0.0387	221	0.0384	0.0	0.0384
473	-0.0306	0.0	0.0306	223	-0.0265	0.0	0.0265
475	0.0307	0.0	0.0307	225	0.0	0.0	0.0
477	-0.0388	0.0	0.0388	227	0.0265	0.0	0.0265
479	0.0	0.0	0.0	229	-0.0383	0.0	0.0383
421	0.0408	0.0052	0.0411	171	0.0033	-0.0658	0.0659
423	0.0047	-0.0427	0.0430	173	0.0719	0.1183	0.1384
425	0.0	0.0480	0.0480	175	-0.0720	0.1183	0.1385
427	-0.0046	-0.0427	0.0429	177	-0.0032	-0.0658	0.0659
429	-0.0407	0.0052	0.0411	179	0.0	0.0426	0.0426
371	0.0266	-0.0634	0.0688	121	-0.0349	-0.0195	0.0400
373	0.0328	0.0051	0.0332	123	0.0816	0.0427	0.0921
375	-0.0328	0.0051	0.0332	125	0.0	0.0284	0.0284
377	-0.0267	-0.0634	0.0688	127	-0.0816	0.0427	0.0921
379	0.0	0.0700	0.0700	129	0.0348	-0.0195	0.0399
321	-0.0349	0.0195	0.0399	71	0.0266	0.0635	0.0689
323	0.0816	-0.0426	0.0921	73	0.0328	-0.0051	0.0332
325	0.0	-0.0285	0.0285	75	-0.0328	-0.0051	0.0332
327	-0.0816	-0.0426	0.0921	77	-0.0267	0.0635	0.0689
329	0.0348	0.0195	0.0399	79	0.0	-0.0700	0.0700
271	0.0033	0.0659	0.0660	21	0.0408	-0.0053	0.0411
273	0.0719	-0.1182	0.1384	23	0.0047	0.0428	0.0430
275	-0.0720	-0.1182	0.1384	25	0.0	-0.0479	0.0479
277	-0.0032	0.0659	0.0660	27	-0.0046	0.0428	0.0430
279	0.0	-0.0427	0.0427	29	-0.0407	-0.0053	0.0411

TABLE XXXI

Uniaxial Compression $\eta = 1.375$: SCV displacement field (DX, DY, DZ) in the $y = 4.5$ plane through the vacancy at site 225. $DY = 0$ for all sites in the $y = 4.5$ plane. DX, DY, and DR are expressed in hlc (xy).

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0496	0.0	0.0496	221	0.0716	0.0	0.0716
473	-0.0667	0.0	0.0667	223	-0.0110	0.0	0.0110
475	0.0668	0.0	0.0668	225	0.0	0.0	0.0
477	-0.0496	0.0	0.0496	227	0.0109	0.0	0.0109
479	0.0	0.0	0.0	229	-0.0716	0.0	0.0716
421	0.0445	0.0182	0.0481	171	0.0245	-0.0863	0.0897
423	-0.0100	-0.0784	0.0790	173	0.0802	0.1022	0.1300
425	0.0	0.0949	0.0949	175	-0.0802	0.1022	0.1299
427	0.0100	-0.0784	0.0790	177	-0.0245	-0.0863	0.0897
429	-0.0444	0.0182	0.0480	179	0.0	0.0878	0.0878
371	0.0036	-0.0784	0.0785	121	-0.0510	0.0040	0.0511
373	0.0500	0.0371	0.0622	123	0.0980	0.0115	0.0987
375	-0.0499	0.0371	0.0622	125	0.0	0.0101	0.0101
377	-0.0035	-0.0784	0.0785	127	-0.0981	0.0115	0.0988
379	0.0	0.0858	0.0858	129	0.0510	0.0040	0.0512
321	-0.0510	-0.0041	0.0512	71	0.0036	0.0784	0.0784
323	0.0980	-0.0116	0.0987	73	0.0500	-0.0372	0.0623
325	0.0	-0.0100	0.0100	75	-0.0499	-0.0372	0.0622
327	-0.0981	-0.0116	0.0988	77	-0.0035	0.0784	0.0784
329	0.0510	-0.0041	0.0512	70	0.0	-0.0857	0.0857
271	0.0245	0.0862	0.0896	21	0.0445	-0.0183	0.0481
273	0.0802	-0.1023	0.1300	23	-0.0100	0.0784	0.0791
275	-0.0802	-0.1023	0.1300	25	0.0	-0.0949	0.0949
277	-0.0245	0.0862	0.0896	27	0.0100	0.0784	0.0791
279	0.0	-0.0879	0.0879	29	-0.0444	-0.0183	0.0480

TABLE XXXII

Uniaxial Compression $\eta = 1.414$: SCV displacement field (DX, DY, DZ) in the $y = 4.5$ plane through the vacancy at site 225. $DY = 0$ for all sites in the $y = 4.5$ plane. DX, DY, and DR are expressed in h/c (xy).

Site	DX	DZ	DR	Site	DX	DZ	DR
471	-0.0012	0.0	0.0012	221	0.0275	0.0	0.0275
473	-0.0052	0.0	0.0052	223	0.0288	0.0	0.0288
475	0.0052	0.0	0.0052	225	0.0	0.0	0.0
477	0.0013	0.0	0.0013	227	-0.0288	0.0	0.0288
479	0.0	0.0	0.0	229	-0.0274	0.0	0.0274
421	0.0233	-0.0199	0.0306	171	0.0238	-0.0246	0.0342
423	-0.0050	0.0061	0.0079	173	0.1022	0.0817	0.1326
425	0.0	0.0156	0.0156	175	-0.1044	0.0817	0.1326
427	0.0051	0.0061	0.0079	177	0.0238	-0.0246	0.0342
429	-0.0233	-0.0199	0.0307	179	0.0	0.0185	0.0185
371	0.0439	-0.0401	0.0658	121	-0.0018	-0.0074	0.0076
373	-0.0010	0.0250	0.0250	123	0.0814	0.0578	0.0998
375	0.0010	0.0250	0.0250	125	0.0	-0.0478	0.0478
377	-0.0439	-0.0491	0.0658	127	-0.0814	0.0578	0.0999
379	0.0	0.0204	0.0204	129	0.0018	-0.0074	0.0076
321	-0.0018	0.0074	0.0076	71	0.0439	0.0491	0.0658
323	0.0814	-0.0578	0.0998	73	-0.0010	-0.0250	0.0250
325	0.0	0.0478	0.0478	75	0.0010	-0.0250	0.0250
327	-0.0814	-0.0578	0.0999	77	-0.0440	0.0491	0.0659
329	0.0018	0.0074	0.0076	79	0.0	-0.0204	0.0204
271	0.0238	0.0246	0.0342	21	0.0232	0.0199	0.0306
273	0.1044	-0.0817	0.1326	23	-0.0050	-0.0061	0.0079
275	-0.1044	-0.0817	0.1346	25	0.0	-0.0156	0.0156
277	-0.0238	0.0246	0.0342	27	0.0051	-0.0061	0.0079
279	0.0	-0.0185	0.0185	29	-0.0233	0.0199	0.0307

TABLE XXXIII

Uniaxial Compression $\eta = 1.50$: SCV displacement field (DX, DY, DZ) in the $y = 4.5$ plane through the vacancy at site 225. $DY \approx 0$ for all sites in the $y = 4.5$ plane. DX, DY, and DR are expressed in h/c (xy).

Site	DX	DZ	DR	Site	DX	DZ	DR
471	-0.0219	0.0	0.0219	221	0.0204	0.0	0.0204
473	-0.0059	0.0	0.0059	223	0.0699	0.0	0.0699
475	0.0060	0.0	0.0060	225	0.0	0.0	0.0
477	0.0219	0.0	0.0219	227	-0.0698	0.0	0.0698
479	0.0	0.0	0.0	229	-0.0204	0.0	0.0204
421	0.0036	-0.0283	0.0285	171	0.0426	0.0118	0.0442
423	-0.0131	0.0179	0.0222	173	0.1144	0.0476	0.1239
425	0.0	0.0176	0.0176	175	-0.1144	0.0476	0.1239
427	0.0130	0.0179	0.0221	177	-0.0427	0.0118	0.0443
429	-0.0035	-0.0283	0.0285	179	0.0	0.0052	0.0052
371	0.0343	0.0302	0.0457	121	0.0211	0.0162	0.0266
373	-0.0108	0.0339	0.0356	123	0.0675	0.0421	0.0796
375	0.0109	0.0339	0.0356	125	0.0	-0.0846	0.0846
377	-0.0344	-0.0302	0.0458	127	-0.0674	0.0421	0.0795
379	0.0	-0.0279	0.0279	129	-0.0212	0.0162	0.0267
321	0.0211	-0.0163	0.0267	71	0.0343	0.0302	0.0457
323	0.0675	-0.0422	0.0796	73	-0.0108	-0.0338	0.0355
325	0.0	0.0845	0.0845	75	0.0109	-0.0338	0.0355
327	-0.0674	0.0422	0.0796	77	-0.0344	0.0302	0.0458
329	-0.0212	-0.0163	0.0267	79	0.0	0.0278	0.0278
271	0.0436	-0.0119	0.0442	21	0.0036	0.0283	0.0285
273	0.1144	-0.0476	0.1239	23	-0.0131	-0.0178	0.0221
275	-0.1144	-0.0476	0.1239	25	0.0	-0.0177	0.0178
277	-0.0698	0.0	0.0698	27	0.0131	-0.0178	0.0221
279	0.0	-0.0051	0.0051	29	-0.0035	0.0283	0.0285

TABLE XXXIV

Angle θ between the line from site 173 to site 225 and the displacement vector direction for the atom at site 173.

η	$\underline{DX}$	$\underline{DY}$	$\underline{\tan \alpha}$	$\underline{\alpha}$	$\underline{\beta}$	$\underline{\theta = \beta - \alpha}$
1.0	0.01	0.01	1.0	45°	45°	0.0°
1.10	0.0188	0.0282	0.667	33.69	47.73	14.04
1.20	0.0474	0.0676	0.701	35.04	50.19	15.15
1.25	0.0619	0.1059	0.584	30.31	51.34	21.03
1.30	0.7200	0.1182	0.609	31.35	52.43	21.08
1.375	0.0802	0.1023	0.784	38.10	53.97	15.87
1.414	0.1044	0.0817	1.278	51.95	54.74	2.79
1.50	0.1144	0.0476	2.403	67.41	56.31	-11.10

$$\alpha = \tan^{-1}(DX/DZ)$$

$$\beta = \cot^{-1} \eta$$

C. Split-Vacancy Displacement Field

Figures 44-52 and Tables XXXV-XLIII describe SV displacement fields. Figure 44 provides two examples of the type of displacement field pattern which correlates with the SV being the vacancy migration saddle-point configuration. Figure 44a is for $\eta = 1.0$ isotropic compression and Fig. 44b is for $\eta = 1.5$ isotropic compression. In both instances, the displacement field pattern is dominated by the displacement vectors of atoms lying on two adjacent $[10\bar{1}]$ lines through the two vacant sites. In addition, the displacement vectors for the atoms at first-neighbor sites 173 and 327 are aligned with the $[101]$ line on which these sites are located. As such, the displacement field pattern is a crossed-axis pattern centered on two crossing close-packed line directions. The acute angle between these lines is 90° and 70.5° , respectively, for an fcc and a bcc crystal. The displacement field of an SV-OP also exhibited a crossed-axis displacement field pattern for $\eta = 1.10$ and $\eta = 1.20$ uniaxial compression. This is shown in Figs. 45 and 46. The acute angle between the crossed axes is 84.5° and 79.6° , respectively, for $\eta = 1.10$ and $\eta = 1.20$. Close inspection of Figs. 45 and 46 shows that uniaxial compression produced a deviation of the first-neighbor displacement vectors toward the compression axis, but the overall pattern is qualitatively a crossed-axis pattern. In particular, atom displacement vectors in the V-regions

between the crossed $[10\bar{1}]$ and $[101]$ axes are small and all displacements tend to point toward the vacant sites.

Figure 47 is a map of the SV-OP displacement field for $\eta = 1.30$ uniaxial compression. The crossed-axis feature seen in Figs. 44-46 is not present in Fig. 47. Instead, the salient pattern feature of the displacement vectors in Fig. 47 is that they tend to be aligned along either the $[101]$ or the $[\bar{1}0\bar{1}]$ direction. This particular alignment feature persists in Fig. 48 for $\eta = 1.375$ uniaxial compression. This alternating-sign, shear displacement pattern for the SV-OP correlates with it being the stable vacancy configuration.

Figure 49 is an SV-OP displacement field map for $\eta = \sqrt{2}$ uniaxial compression (bcc structure). Because the crystal exhibits cubic symmetry, the SCV is the stable configuration. The crossed-axis displacement pattern clearly exists in this instance and, as stated in Sec. IV, the split-vacancy is the saddle-point configuration for $\eta = \sqrt{2}$ uniaxial compression.

The $\eta = 1.5$ uniaxial compression run either was computationally unstable or reveals yet a third qualitatively distinct displacement field pattern for uniaxial compression. The available evidence appears to support the computational instability interpretation.

Figure 50 is a map of the SV-OP displacement field for $\eta = 1.5$ uniaxial compression at the seventh of 20 macro time steps* in the displacement field run for 1.5 compression. As it stands, this displacement field pattern resembles the crossed-axis, bcc crystal structure map of Fig. 49. At the end of the run, however, the displacement field map was that shown in Fig. 51. This "keyhole" pattern is certainly different from the other patterns encountered. Taken together with Fig. 50, it suggests that roughly half of the displacement field follows the crossed-axis model and that the remaining half follows a "circular" pattern, in an xz-plane projection. Note that with only three exceptions, sites 227, 327, and 277, all displacement x-components are positive. In the planes $y = 3.5$ and $y = 5.5$ on either side of the $y = 4.5$ plane, all displacement x-components are negative, and in planes $y = 2.5$ and $y = 6.5$ all displacement x-components are positive. Figure 52 shows the xy-plane projection of displacements for each line $z = \text{constant}$ in the $y = 4.5$ plane. Note that as one moves downward from $z = 9.5$

*The MOLDY program run on which this section is based ran for 200 time steps. In each instance, a macro time step is equal to 10 time steps. Atom position output was printed at the end of each of 20 macro time steps.

to $z = 0.5$, the y -components of the first two and the last two displacements in each line are in a direction opposite to that occurring in each adjacent atom line.

A complete set of SV-IP displacement field tables and maps is not shown in this report because it appears as if the SV-IP does not play a significant role in vacancy migration in a uniaxially compressed crystal. Figures 53-56 are SV-IP displacement field maps for uniaxial compression $\eta = 1.5$.

Figure 53 pertains to the $z = 4.5$ plane in which the split-vacancy perturbation center was located. Figures 54 and 55 describe the displacement field in the $z = 5.5$ and $z = 6.5$ planes. Note the stagnation points at sites 314 and 337 in Figure 55. Atom displacements in the (101) plane, which contains the atom located midway between vacant sites 225 and 226, are plotted in Fig. 56. These four maps are the only ones which were constructed for an in-plane vacancy.

Fig. 44a.
SV displacement field in
the $y = 4.5$ plane. Iso-
tropic compression equal
to 1.0.

Fig. 44b.
SV displacement field in
the $y = 4.5$ plane. Iso-
tropic compression equal
to 1.50.

Fig. 45.
SV-OP displacement field
in the $y = 4.5$ plane.
Uniaxial compression
equal to 1.10.

Fig. 46.
SV-OP displacement field
in the $y = 4.5$ plane.
Uniaxial compression
equal to 1.20.

Fig. 47.
SV-OP displacement field
in the $y = 4.5$ plane.
Uniaxial compression
equal to 1.30.

Fig. 48.
SV-OP displacement field
in the $y = 4.5$ plane.
Uniaxial compression
equal to 1.375.

Fig. 49.
SV-OP displacement field
in the $y = 4.5$ plane.
Uniaxial compression
equal to 1.414.

Fig. 50.
SV-OP displacement field
in the $y = 4.5$ plane.
Uniaxial compression
equal to 1.50. Seventh
iteration, prior to com-
putational instability.

Fig. 51.
SV-OP displacement field
in the $y = 4.5$ plane.
Uniaxial compression
equal to 1.50. Twentieth
iteration.

Fig. 52.

The x- and y-displacements for each z = constant line in the y = 4.5 displacement map for uniaxial compression equal to 1.50.

TABLE XXXV

Isotropic Compression $\eta = 1.0$: SV displacement field (DX, DY, DZ) in the $y = 4.5$ plane. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in hlc units. DY = 0 for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0005	0.0001	0.0005	221	0.0005	0.0004	0.0006
473	0.0005	-0.0002	0.0005	223	0.0030	0.0034	0.0045
475	-0.0004	-0.0004	0.0006	225	0.5	0.5	0.7071
477	-0.0006	-0.0006	0.0010	227	-0.0294	0.0118	0.0317
479	-0.0003	-0.0003	0.0004	229	-0.0014	-0.0009	0.0014
421	-0.0001	-0.0004	0.0004	171	0.0016	0.0016	0.0023
423	0.0015	-0.0010	0.0018	173	0.0095	0.0095	0.0134
425	-0.0003	-0.0014	0.0014	175	-0.0117	0.0294	0.0316
427	-0.0017	-0.0017	0.0024	177	-0.0056	0.0048	0.0074
429	-0.0013	-0.0013	0.0018	179	-0.0002	0.0005	0.0005
371	0.0010	-0.0014	0.0017	121	0.0005	0.0008	0.0009
373	0.0048	-0.0057	0.0074	123	0.0036	0.0036	0.0051
375	-0.0034	-0.0030	0.0045	125	0.0034	0.0030	0.0045
377	-0.0035	-0.0035	0.0049	127	-0.0048	0.0057	0.0074
379	---	---	---	129	-0.0010	0.0015	0.0018
321	0.0002	-0.0006	0.0006	71	0.0012	0.0012	0.0017
323	0.0057	-0.0048	0.0074	73	0.0016	0.0016	0.0023
325	0.0118	-0.0294	0.0317	75	0.0003	0.0015	0.0015
327	-0.0095	-0.0095	0.0134	77	-0.0014	0.0010	0.0017
329	-0.0017	-0.0017	0.0024	79	0.0001	0.0005	0.0005
271	0.0015	0.0003	0.0015	21	0.0003	0.0003	0.0004
273	0.0294	-0.0117	0.0316	23	0.0008	0.0005	0.0009
275	0.0	0.0	0.0	25	0.0004	0.0005	0.0006
277	-0.0030	-0.0034	0.0045	27	-0.0006	0.0002	0.0006
279	-0.0004	-0.0004	0.0006	29	-0.0004	-0.0001	0.0004

TABLE XXXVI

Isotropic Compression $\eta = 1.5$: SV displacement field (DX, DY, DZ) in the $y = 4.5$ plane. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in the hlc units. $DY = 0$ for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0039	-0.0014	0.0041	221	0.0015	0.0016	0.0022
473	0.0036	-0.0018	0.0040	223	0.0126	0.0063	0.0141
475	-0.0015	-0.0016	0.0022	225	0.5	0.5	0.7071
477	-0.0048	-0.0022	0.0053	227	-0.0543	0.0309	0.0625
479	-0.0019	-0.0019	0.0027	229	-0.0059	0.0019	0.0062
421	0.0015	-0.0038	0.0041	171	0.0064	0.0062	0.0089
423	0.0073	-0.0063	0.0096	173	0.0374	0.0374	0.0529
425	0.0019	-0.0058	0.0061	175	-0.0308	0.0542	0.0623
427	-0.0062	-0.0064	0.0089	177	-0.0166	0.0150	0.0224
429	-0.0066	-0.0066	0.0093	179	-0.0018	0.0036	0.0040
371	0.0064	-0.0074	0.0098	121	0.0022	0.0049	0.0054
373	0.0150	-0.0166	0.0224	123	0.0152	0.0152	0.0215
375	-0.0062	-0.0126	0.0140	125	0.0063	0.0126	0.0141
377	-0.0152	-0.0152	0.0215	127	-0.0151	0.0165	0.0224
379	-0.0022	-0.0048	0.0053	129	-0.0063	0.0073	0.0096
321	0.0018	-0.0036	0.0040	71	0.0067	0.0067	0.0095
323	0.0165	-0.0151	0.0224	73	0.0062	0.0064	0.0089
325	0.0309	-0.0543	0.0625	75	-0.0018	0.0059	0.0062
327	-0.0375	-0.0375	0.0530	77	-0.0074	0.0064	0.0098
329	-0.0064	-0.0062	0.0089	79	-0.0014	0.0039	0.0041
271	0.0059	-0.0018	0.0062	21	0.0020	0.0020	0.0028
273	0.0542	-0.0308	0.0623	23	0.0049	0.0022	0.0054
275	0.0	0.0	0.0	25	0.0016	0.0015	0.0022
277	-0.0126	-0.0062	0.0140	27	-0.0036	0.0018	0.0040
279	-0.0016	-0.0015	0.0022	29	-0.0038	0.0015	0.0041

TABLE XXXVII

Uniaxial Compression $\eta = 1.10$: SV-OP displacement field (DX, DY, DZ) in the $y = 4.5$ plane. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in hlc units. $DY = 0$ for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0044	-0.0009	0.0045	221	-0.0002	0.0	0.0002
473	0.0034	-0.0019	0.0039	223	-0.0009	0.0051	0.0052
475	-0.0010	-0.0009	0.0013	225	0.5	0.4545	0.6757
477	-0.0047	-0.0017	0.0050	227	-0.0458	0.0417	0.0619
479	-0.0020	-0.0014	0.0024	229	0.0013	-0.0007	0.0015
421	0.0026	-0.0017	0.0031	171	0.0008	0.0014	0.0016
423	0.0071	-0.0056	0.0090	173	0.0283	0.0423	0.0509
425	0.0024	-0.0053	0.0058	175	-0.0240	0.0463	0.0522
427	-0.0048	0.0463	0.0522	177	-0.0150	0.0163	0.0222
429	-0.0069	-0.0053	0.0087	179	0.0003	-0.0004	0.0005
371	0.0063	-0.0059	0.0086	121	0.0006	0.0001	0.0006
373	0.0142	-0.0155	0.0210	123	0.0143	0.0149	0.0206
375	-0.0030	-0.0107	0.0111	125	0.0030	0.0106	0.0110
377	-0.0144	-0.150	0.0208	127	-0.0143	0.0156	0.0212
379	-0.0007	-0.0001	0.0007	129	-0.0062	0.0058	0.0085
321	-0.0002	0.0004	0.0004	71	0.0070	0.0052	0.0087
323	0.0150	-0.0165	0.0223	73	0.0048	0.0054	0.0072
325	0.0241	-0.0464	0.0522	75	-0.0024	0.0054	0.0059
327	-0.0283	0.0424	0.0510	77	-0.0071	0.0056	0.0090
329	-0.0007	-0.0014	0.0016	79	-0.0029	0.0016	0.0031
271	-0.0012	0.0006	0.0013	21	0.0020	0.0015	0.0025
273	0.0459	-0.0417	0.0620	23	0.0047	0.0016	0.0050
275	0.0	0.0	0.0	25	0.0010	0.0008	0.0013
277	0.0008	-0.0050	0.0051	27	-0.0034	0.0018	0.0038
279	0.0001	0.0	0.0001	29	-0.0044	0.0008	0.0045

TABLE XXXVIII

Uniaxial Compression $\eta = 1.20$: SV-OP displacement field (DX, DY, DZ) in the $y = 4.5$ plane. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in hlc units. $DY = 0$ for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0122	0.0023	0.0124	221	0.0008	-0.0013	0.0015
473	0.0054	-0.0067	0.0086	223	-0.0094	-0.0028	0.0098
475	0.0003	0.0028	0.0028	225	0.5	0.4167	0.6509
477	-0.0133	-0.0050	0.0142	227	-0.0665	0.0875	0.1099
479	-0.0060	-0.0056	0.0082	229	0.0022	-0.0076	0.0079
421	0.0122	0.0026	0.0125	171	-0.0038	-0.0124	0.0130
423	0.0111	-0.0102	0.0151	173	0.0587	0.0894	0.1069
425	0.0072	-0.0062	0.0095	175	-0.0089	0.0444	0.0453
427	-0.0114	-0.0112	0.0160	177	-0.0335	0.0292	0.0444
429	-0.0341	-0.0161	0.0282	179	0.0027	-0.0071	0.0076
371	0.0163	-0.0126	0.0206	121	-0.0023	-0.0138	0.0140
373	0.0180	-0.0152	0.0236	123	0.0392	0.0384	0.0549
375	-0.0049	-0.0202	0.0208	125	0.0050	0.0203	0.0209
377	-0.0393	-0.0383	0.0549	127	-0.0180	0.0152	0.0236
379	0.0022	0.0138	0.0140	129	-0.0163	0.0125	0.0205
321	-0.0026	0.0072	0.0076	71	0.0231	0.0162	0.0282
323	0.0336	-0.0292	0.0445	73	0.0115	0.0112	0.0160
325	0.0089	-0.0445	0.0454	75	-0.0072	0.0062	0.0095
327	-0.0587	-0.0895	0.1070	77	-0.0110	0.0102	0.0150
329	0.0038	0.0125	0.0131	79	-0.0122	-0.0027	0.0125
271	-0.0022	0.0075	0.0078	21	0.0060	0.0055	0.0081
273	0.0665	-0.0874	0.1098	23	0.0132	0.0051	0.0142
275	0.0	0.0	0.0	25	-0.0002	-0.0028	0.0028
277	0.0095	0.0032	0.0100	27	-0.0054	0.0066	0.0085
279	-0.0007	0.0014	0.0016	29	-0.0123	-0.0024	0.0125

TABLE XXXIX

Uniaxial Compression $\eta = 1.25$: SV-OP displacement field (DX, DY, DZ) in the $y = 4.5$ plane. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in hlc units. DY = 0 for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0248	0.0083	0.0262	221	0.0064	0.0027	0.0069
473	0.0014	-0.0108	0.0109	223	-0.0127	-0.0260	0.0289
475	0.0036	0.0083	0.0090	225	0.5	0.4	0.6403
477	-0.0212	-0.0157	0.0264	227	-0.0642	0.1016	0.1202
479	-0.0130	-0.0050	0.0139	229	-0.0061	-0.0129	0.0143
421	0.0201	0.0218	0.0296	171	-0.0114	-0.0352	0.0370
423	0.0106	-0.0198	0.0225	173	0.0830	0.1075	0.1358
425	0.0095	-0.0063	0.0095	175	0.0043	0.0430	0.0432
427	-0.0192	-0.0194	0.0273	177	-0.0413	0.0216	0.0466
429	-0.0356	-0.0310	0.0472	179	0.0056	-0.0034	0.0066
371	0.0131	-0.0138	0.0190	121	-0.0125	-0.0327	0.0350
373	0.0217	-0.0106	0.0242	123	0.0600	0.0590	0.0841
375	-0.0130	-0.0240	0.0273	125	0.0130	0.0238	0.0271
377	-0.0600	-0.0589	0.0841	127	-0.0216	0.0106	0.0241
379	0.0124	0.0327	0.0350	129	-0.0130	0.0137	0.0189
321	-0.0056	0.0034	0.0066	71	0.0356	0.0310	0.0472
323	0.0412	-0.0216	0.0465	73	0.0191	0.0194	0.0272
325	-0.0042	-0.0430	0.0432	75	-0.0095	0.0002	0.0095
327	-0.0831	-0.1074	0.1358	77	-0.0106	0.0198	0.0224
329	0.0113	0.0351	0.0369	79	-0.0201	-0.0218	0.0296
271	0.0061	0.0128	0.0142	21	0.0131	0.0049	0.0140
273	0.0642	-0.1016	0.1202	23	0.0211	0.0158	0.0264
275	0.0	0.0	0.0	25	-0.0036	-0.0084	0.0091
277	0.0126	0.0261	0.0290	27	-0.0014	0.0108	0.0109
279	-0.0065	-0.0026	0.0070	29	-0.0248	-0.0084	0.0262

TABLE XL

Uniaxial Compression $\eta = 1.375$: SV-OP displacement field (DX, DY, DZ) in the $y = 4.5$ plane. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in hlc units. $DY = 0$ for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0578	0.0220	0.0618	221	0.0658	-0.0768	0.1011
473	-0.0661	-0.0767	0.1012	223	0.0012	0.0688	0.0688
475	0.0569	0.0853	0.1025	225	0.5	0.3636	0.6182
477	-0.0296	-0.0533	0.0610	227	-0.0404	0.0751	0.0852
479	-0.0365	0.0092	0.0376	229	-0.0748	-0.0766	0.1070
421	0.0238	0.0882	0.0913	171	-0.0195	-0.0711	0.0737
423	-0.0441	-0.1059	0.1147	173	0.1321	0.1029	0.1674
425	0.0463	0.0945	0.1052	175	0.0226	0.0151	0.0272
427	-0.0349	-0.0279	0.0447	177	-0.0783	-0.0787	0.1109
429	-0.0423	-0.0594	0.0729	179	0.0510	0.0913	0.1046
371	-0.0633	-0.0646	0.0904	121	-0.0394	-0.0583	0.0704
373	0.0686	0.0767	0.1029	123	0.0883	-0.0747	0.1156
375	-0.0372	0.0028	0.0373	125	0.0372	-0.0028	0.0373
377	-0.0884	-0.0747	0.1157	127	-0.0687	-0.0767	0.1030
379	0.0393	0.0583	0.0703	129	0.0633	0.0646	0.0904
321	-0.0510	-0.0913	0.1046	71	0.0422	0.0594	0.0729
323	0.0784	0.0786	0.1110	73	0.0350	0.0279	0.0448
325	-0.0226	-0.0151	0.0272	75	-0.0464	-0.0945	0.1053
327	-0.1322	-0.1031	0.1676	77	0.0441	0.1059	0.1147
329	0.0195	0.0711	0.0737	79	-0.0238	-0.0881	0.0913
271	0.0749	0.0767	0.1072	21	0.0364	-0.0094	0.0376
273	0.0403	-0.0751	0.0852	23	0.0296	0.0533	0.0610
275	0.0	0.0	0.0	25	-0.0568	-0.0855	0.1026
277	-0.0011	0.0688	0.0688	27	0.0662	0.0767	0.1013
279	-0.0658	-0.0768	0.1011	29	-0.0577	-0.0220	0.0618

TABLE XLI

Uniaxial Compression $\eta = 1.414$: SV-OP displacement field (DX, DY, DZ) in the $y = 4.5$ plane. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in the hlc units. $DY = 0$ for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	-0.0100	0.0033	0.0105	221	0.0152	0.0066	0.0166
473	0.0002	-0.0032	0.0032	223	0.0423	-0.0072	0.0429
475	0.0	0.0081	0.0081	225	0.5	0.3536	0.6124
477	0.0048	0.0188	0.0194	227	-0.1161	0.0584	0.1300
479	-0.0040	-0.0284	0.0286	229	-0.0273	-0.0095	0.0289
421	0.0160	-0.0165	0.0230	171	0.0221	-0.0160	0.0273
423	-0.0016	0.0037	0.0040	173	0.1238	0.0969	0.1572
425	-0.0007	0.0068	0.0068	175	-0.0219	-0.0399	0.0455
427	0.0095	0.0269	0.0285	177	-0.0660	0.0363	0.0753
429	-0.0526	-0.0443	0.0688	179	0.0020	0.0017	0.0026
371	0.0313	-0.0318	0.0446	121	0.0083	-0.0157	0.0178
373	0.0078	0.0123	0.0146	123	0.0889	0.0759	0.1169
375	0.0108	0.0492	0.0504	125	-0.0107	-0.0492	0.0504
377	-0.0888	-0.0762	0.1170	127	-0.0079	-0.0124	0.0147
379	-0.0084	0.0158	0.0179	129	-0.0313	0.0318	0.0446
321	-0.0020	-0.0017	0.0026	71	0.0524	0.0443	0.0686
323	0.0659	-0.0365	0.0753	73	-0.0094	-0.0269	0.0285
325	0.0219	0.0399	0.0455	75	0.0006	-0.0068	0.0068
327	-0.1239	-0.0969	0.1573	77	0.0017	-0.0038	0.0042
329	-0.0221	0.0160	0.0273	79	-0.0160	0.0167	0.0231
271	0.0272	0.0096	0.0288	21	0.0039	0.0283	0.0286
273	0.1161	-0.0584	0.1300	23	-0.0048	-0.0187	0.0193
275	0.0	0.0	0.0	25	-0.0001	-0.0082	0.0082
277	-0.0424	0.0074	0.0430	27	-0.0001	0.0034	0.0034
279	-0.0152	-0.0066	0.0166	29	0.0100	-0.0032	0.0105

TABLE XLII

Uniaxial Compression $\eta = 1.50$: SV-OP displacement field (DX, DY, DZ) in the $y = 4.5$ plane at the seventh macro time step. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in hlc units. $DY = 0$ for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	-0.0149	-0.0023	0.0151	221	0.0131	0.0012	0.0132
473	-0.0080	0.0011	0.0081	223	0.0737	0.0077	0.0741
475	0.0037	0.0146	0.0151	225	0.5	0.3333	0.6009
477	0.0153	0.0135	0.0204	227	-0.1449	0.0400	0.1503
479	0.0011	-0.0204	0.0204	229	-0.0380	0.0070	0.0386
421	0.0076	-0.0261	0.0272	171	0.0387	0.0103	0.0400
423	-0.0015	0.0050	0.0052	173	0.1156	0.0614	0.1309
425	-0.0036	0.0170	0.0174	175	-0.0373	-0.0734	0.0823
427	0.0157	0.0318	0.0355	177	-0.0708	0.0394	0.0810
429	-0.0287	-0.0312	0.0424	179	-0.0105	0.0083	0.0134
371	0.0339	-0.0283	0.0422	121	0.0125	0.0131	0.0181
373	0.0092	0.0154	0.0179	123	0.0664	0.0478	0.0818
375	0.0149	0.0731	0.0746	125	-0.0148	-0.0731	0.0746
377	-0.0663	-0.0478	0.0817	127	-0.0090	-0.0154	0.0178
379	-0.0125	-0.0132	0.0182	129	-0.0337	0.0284	0.0441
321	0.0107	-0.0082	0.0135	71	0.0288	0.0311	0.0424
323	0.0709	-0.0395	0.0812	73	-0.0157	-0.0318	0.0355
325	0.0374	0.0734	0.0824	75	0.0037	-0.0170	0.0174
327	-0.1155	-0.0613	0.1308	77	0.0017	-0.0051	0.0054
329	-0.0386	-0.0104	0.0400	79	-0.0075	0.0262	0.0272
271	0.0382	-0.0071	0.0388	21	-0.0009	0.0205	0.0205
273	0.1450	-0.0400	0.1504	23	-0.0152	-0.0136	0.0204
275	0.0	0.0	0.0	25	-0.0036	-0.0146	0.0150
277	-0.0735	-0.0078	0.0739	27	0.0081	-0.0010	0.0082
279	-0.0129	-0.0012	0.0130	29	0.0150	0.0022	0.0152

TABLE XLIII

Uniaxial Compression $\eta = 1.50$: SV-OP displacement field (DX, DY, DZ) in the $y = 4.5$ plane at the 20th macro time step. Sites 225 and 275 are vacant. The atom initially at site 225 is located at (5.0, 4.5, 5.0) in hlc units. $DY = 0$ for all sites in the $y = 4.5$ plane.

Site	DX	DZ	DR	Site	DX	DZ	DR
471	0.0370	-0.0207	0.0424	221	0.0709	0.0306	0.0772
473	0.0432	-0.0025	0.0433	223	0.1075	0.0202	0.1094
475	0.0676	0.0194	0.0703	225	0.5	0.3333	0.6009
477	0.0706	0.0226	0.0741	227	-0.0858	0.0273	0.0900
479	0.0619	-0.0122	0.0631	229	0.0184	0.0035	0.0187
421	0.0554	-0.0368	0.0665	171	0.0897	0.0220	0.0924
423	0.0507	-0.0050	0.0509	173	0.1375	0.0604	0.1502
425	0.0546	0.0223	0.0590	175	0.0031	-0.0645	0.0646
427	0.0745	0.0388	0.0840	177	-0.0065	0.0219	0.0228
429	0.0339	-0.0218	0.0403	179	0.0513	0.0138	0.0531
371	0.0783	-0.0283	0.0832	121	0.0754	0.0286	0.0806
373	0.0610	0.0155	0.0629	123	0.1050	0.0441	0.1139
375	0.0738	0.0797	0.1086	125	0.0289	-0.0709	0.0766
377	-0.0024	-0.0361	0.0362	127	0.0392	-0.0120	0.0410
379	0.0399	-0.0270	0.0482	129	0.0339	0.0209	0.0398
321	0.0641	-0.0138	0.0656	71	0.0797	0.0326	0.0861
323	0.1088	-0.0290	0.1126	73	0.0286	-0.0375	0.0472
325	0.0820	0.0868	0.1194	75	0.0562	-0.0178	0.0590
327	-0.0587	-0.0590	0.0832	77	0.0537	0.0042	0.0539
329	0.0137	-0.0205	0.0247	79	0.0646	0.0312	0.0717
271	0.0839	-0.0019	0.0839	21	0.0653	0.0174	0.0676
273	0.1737	-0.0253	0.1755	23	0.0289	-0.0222	0.0364
275	0.0	0.0	0.0	25	0.0524	-0.0167	0.0550
277	-0.0206	-0.0154	0.0257	27	0.0659	0.0065	0.0662
279	0.0450	-0.0058	0.0454	29	0.0718	0.0163	0.0736

Fig. 53.
SV-IP displacement field in the $z = 4.5$ plane. Uniaxial compression equal to 1.50.

Fig. 54.
SV-IP displacement field in the $z = 5.5$ plane. Uniaxial compression equal to 1.50.

Fig. 55.
SV-IP displacement field
in the $z = 6.5$ plane. Uni-
axial compression equal
to 1.50.

Fig. 56.
SV-IP displacement field in
the (110) plane through the
midpoint atom. Uniaxial com-
pression equal to 1.50.

VI. SUMMARY AND CONCLUSIONS

This study consisted of running static equilibrium calculations for a vacancy in an fcc Lennard-Jones crystal subjected to (1) isotropic compression in one instance, and (2) uniaxial compression along the [001] axis in the second instance. The SCV and SV configurations were considered in the case of isotropic compression. Three vacancy configurations were studied in the case of uniaxial compression; these were the SCV, SV-IP, and SV-OP. The compression ranges considered for isotropic compression and uniaxial compression were $0.94 \leq \eta \leq 1.50$ and $1.0 \leq \eta \leq 1.5$, respectively.

The purposes of the study were (1) to characterize vacancy migration in a uniaxially compressed crystal for use in interpreting shock process simulation results for a crystal containing vacancy defects, and (2) to identify seeming defect displacement field "properties" that might be artifacts of imposing periodic boundary conditions in the computer experiments. In general, a computer experiment study of defect migration involves (1) discovering what is the stable defect configuration, and (2) discovering what is the saddle-point configuration for the migration of the defect.

If the involved defect is a point defect, one usually can guess what is the stable defect configuration and can reduce the number of saddle-point possibilities to two or three on the basis of crystal symmetry. If, however, the defect is not a point defect, there is currently no way to determine uniquely either the stable defect configuration or the saddle-point configuration. Because of these circumstances, the initial exploration of either a vacancy or an interstitial defect proceeds on the assumption that the defect will, in fact, behave like a point defect. This tactic normally is profitable in the sense that it usually gives a qualitatively correct picture of the "actual" migration process, even though the defect concerned is not properly a point defect.

A light-hearted definition of a point defect is: A point defect is a defect that is easy to work with in a computer experiment. In many ways this statement is close to the truth. Let us call the part of a defect displacement field in which the atom displacements are greater than or equal to 1% of the interatomic distance the GE1% displacement field. From experience we know that defect migration calculations normally are difficult when the defect's GE1% displacement field exceeds 100 av, where av stands for atomic volume. This is true because a migration calculation ultimately reduces to potential energy surface mapping and when the defect displacement field is extensive, each of a myriad atom-position

arrangements will correspond to a given crystal energy stipulation. In effect, a defect is a point defect if one can characterize its migration process by characterizing the movement of a single atom in the defect core. When the movement of two or more atoms in the defect core needs to be characterized in a migration calculation, the defect is, in effect, an extended defect and is intractable.

In the case of the fcc Lennard-Jones crystal concerned, it was found that the stable vacancy configuration is a function of the uniaxial compression magnitude. For $1.0 \leq \eta \leq 1.29$, the SCV is the stable configuration, and for $1.29 \leq \eta \leq 1.5$, the SV-OP is the stable configuration. The SV-IP was not found to be the stable vacancy configuration in any of the uniaxial compression runs. In the case of isotropic compression, the SCV was the stable vacancy configuration for $0.94 \leq \eta \leq 1.5$.

Purely repulsive atom pair-potential energy functions were used in many of the early computer experiments on defect properties. In particular, Vineyard (1961) shows pictures of the vacancy cluster configurations that are predicted when a purely repulsive atom pair interaction is assumed. In each of these examples, the vacancy cluster configuration energy is lowered by the intrusion of atoms, initially at the cluster surface, into the central portion of an initially empty, compact void. One example is a divacancy configuration in an fcc crystal that consists of four vacant atom sites at the corners of a tetrahedron, inside of which are located two intruded atoms. A similar effect occurs in the case of the SV-OP. In this instance, we have two vacant sites with an atom between them. The intruded atom feature of vacancy defects when the atom interaction is repulsive is part, but not all, of the reason for the SV-OP becoming the stable vacancy configuration. It cannot be the only reason because the SCV still is the stable vacancy form in isotropic compression at $\eta = 1.5$. The repulsive interaction, intruded atom effect is assisted by the asymmetry provided by uniaxial compression. The resolved stress along $\pm[101]$ provides forces that induce atom shear displacements favorable to SV-OP formation.

As shown in Fig. 43, the angle θ between the displacement vector for an atom at a first-neighbor site of an SCV and the $\langle 110 \rangle$ line connecting that site with the vacant site center increases with uniaxial compression from zero, at $\eta = 1.0$, to 21.1° at $\eta = 1.275$. This increase corresponds to a displacement vector swing toward the $[001]$ compression axis. For $1.275 \leq \eta \leq 1.425$, θ decreases from 21.1° to zero and then falls to -11.1° at $\eta = 1.5$. The negative progression corresponds to a swing from the $\langle 110 \rangle$ site-to-site line direction toward

the basal plane. The onset of the displacement vector rotation away from the stress axis toward the basal plane at $\eta = 1.275$ correlates closely with the compression, $\eta = 1.286$, at which the SV-OP becomes the stable vacancy configuration.

The SV-OP displacement field pattern changes from the so-called crossed-axis pattern, exemplified in Figs. 44-46, to an alternating sign [101] shear pattern, exemplified by Figs. 47 and 48, as the uniaxial compression increases from 1.20 to 1.375. This compression range (centered on 1.30), in which the alternating sign, shear pattern develops, coincides with the compression range in which the SCV first-neighbor atom displacement vectors move away from the stress axis direction and toward the basal plane. In addition, it also coincides with the compression range in which the vacancy migration energy falls to a minimum at $\eta = 1.30$, as shown in Fig. 22.

It appears that a vacancy in a uniaxially compressed crystal is an extended defect for $\eta > 1.20$. The alternating sign [101], shear displacement, field aspect of the vacancy displacement field is sufficiently developed for $\eta > 1.20$ that the displacement field nearly fills the computational cell. Tables XLIV and XLV describe the expansion of the vacancy displacement field that occurs with increasing uniaxial compression. Table XLIV pertains to the SCV and Table XLV to the SV-OP. Each of the uniaxial compression displacement field maps and tables in Sec. V pertains to the $y = 4.5$ plane in the computational cell--the plane in which the vacancy was located. Tables XLIV and XLV list the numbers of sites in a $y = 4.5$ plane that are in the vacancy GE1% and GE3% displacement fields. In the case of the SCV, these numbers include the vacant site, site 225, and in the case of the SV-OP, they include vacant sites 225 and 275. For $\eta > 1.20$, the fraction of the $y = 4.5$ plane sites in either the GE1% or GE3% displacement field is a good estimate of the fraction of all sites in the computational cell in either the GE1% or GE3% displacement field. These fractions are enclosed with parentheses in Tables XLIV and XLV.

Tables XLIV and XLV, together with the displacement field map figures for uniaxial compression $\eta > 1.2$ clearly show that the vacancy displacement field fills the computational cell for $\eta > 1.2$. As such, the volume of the vacancy displacement field region is 400-500 av, and the vacancy behaves like an extended defect (that is, its migration cannot be characterized by characterizing the movement of a single core atom). Part of the extended defect character indicated by the calculations may be an artifact of using periodic boundary conditions,

TABLE XLIV

Number of atoms in the $y = 4.5$ plane in the GE1% and GE3% displacement fields of an SCV at site 225 as a function of uniaxial compression, η .

Compression	GE1%	GE3%
1.0	5 (0.10)	0
1.20	18 (0.36)	8 (0.16)
1.25	41 (0.82)	12 (0.24)
1.30	49 (0.98)	26 (0.52)
1.375	45 (0.90)	45 (0.90)
1.414	37 (0.74)	13 (0.26)
1.50	45 (0.90)	20 (0.40)

TABLE XLV

Number of atoms in the $y = 4.5$ plane in the GE1% and GE3% displacement fields of an SV-OP as a function of uniaxial compression, η . Vacancies are at sites 225 and 275.

Compression	GE1%	GE3%
1.10	15 (0.30)	8 (0.16)
1.20	28 (0.56)	11 (0.22)
1.25	39 (0.78)	12 (0.24)
1.375	50 (1.00)	43 (0.86)
1.414	38 (0.76)	19 (0.38)
1.50	42 (0.84)	18 (0.36)

but in any event, we know that the vacancy displacement field cannot be encompassed by a 500-site computational cell for uniaxial compression $\eta > 1.2$.

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APPENDIX A
DISCONTINUITIES IN THE PERFECT CRYSTAL ENERGY
VERSUS COMPRESSION CURVE

Compression causes each neighbor shell radius $r_n(\eta)$ to diminish as η increases. Because the Lennard-Jones interatomic potential was truncated at $r_{\text{cut}} = 2.73823 \text{ hlc(xy)}$, a discontinuity in the crystal energy occurs whenever an $r_n(\eta)$ falls below r_{cut} due to an increase in compression.

I. ISOTROPIC COMPRESSION

A. Fourth Neighbors

$$r_4(\eta) = \left(0 + \frac{4}{x^2} + \frac{4}{x^2}\right)^{1/2}, \quad \text{where } x = \eta^{1/3}.$$

$$r_4(\eta)^2 = \frac{8}{x^2}.$$

Setting $r_4(\eta)^2 = r_{\text{cut}}^2$ gives $x = 1.032940$ and $\eta = x^3 = 1.102111$. Hence, $r_4(\eta)$ will be less than r_{cut} for all $\eta > \eta_4 = 1.102111$.

B. Fifth Neighbors

$$r_5(\eta) = \left(0 + \frac{1}{x^2} + \frac{9}{x^2}\right)^{1/2}, \quad \text{where } x = \eta^{1/3}.$$

$$r_5(\eta)^2 = \frac{10}{x^2}.$$

Setting $r_5(\eta)^2 = r_{\text{cut}}^2$ gives $x = 1.154862$ and $\eta_5 = x^3 = 1.540246$.

II. UNIAXIAL COMPRESSION

A. Fourth Neighbor Subshell (022)

$$r_4(\eta) = \left(0 + 4 + \frac{4}{\eta^2}\right)^{1/2}.$$

Setting $r_4(\eta)^2 = r_{\text{cut}}^2$ gives $2.738230^2 - 4 = 4/\eta^2$. $\eta_4 = 1.069365$.

B. Fifth Neighbor Subshell (013)

$$r_5(\eta) = \left(0 + 1 + \frac{9}{\eta^2}\right)^{1/2} .$$

Setting $r_5(\eta)^2 = r_{\text{cut}}^2$ gives $\eta_5 = 1.176887$ for (013) fifth neighbors.

C. Fifth Neighbor Subshell (031)

$$r_5(\eta) = \left(0 + 9 + \frac{1}{\eta^2}\right)^{1/2} .$$

$$r_5(\eta)^2 \geq 9 > r_{\text{cut}}^2 \text{ for all } \eta .$$

D. Sixth Neighbors

$$r_6(\eta) = \left(4 + 4 + \frac{4}{\eta^2}\right)^{1/2} .$$

$$r_6(\eta)^2 \geq 8 > r_{\text{cut}}^2 \text{ for all } \eta .$$

E. Seventh Neighbor Subshell (123)

$$r_7(\eta) = \left(1 + 4 + \frac{9}{\eta^2}\right)^{1/2} .$$

Setting $r_7(\eta)^2 = r_{\text{cut}}^2$ gives $\eta_7 = 2.449832$.

F. Seventh Neighbor Subshell (132)

$$r_7(\eta) = \left(1 + 9 + \frac{1}{\eta^2}\right)^{1/2} > r_{\text{cut}} \text{ for all } \eta .$$

G. Seventh Neighbor Subshell (231)

$$r_7(\eta) = \left(4 + 9 + \frac{1}{\eta^2}\right)^{1/2} > r_{\text{cut}} \text{ for all } \eta .$$

H. Eighth Neighbor Subshell (004)

$$r_8(\eta) = \left(\frac{16}{\eta^2}\right)^{1/2}.$$

Setting $r_8(\eta)^2 = r_{\text{cut}}^2$ gives $\eta_8 = 1.460798$.

Note: Distance is expressed in basal plane hlc(xy) in the above calculations. The basal plane hlc is denoted as hlc*.

APPENDIX B

VACANCY RELAXATION COMPUTATION: INITIAL RANDOM ATOM DISPLACEMENTS

This appendix gives the initial random atom displacements for the first neighbors of the vacancy in the site-centered vacancy computation for $\eta = 1.0$. The displacements are expressed in hlc.

<u>Site</u>	<u>DX</u>	<u>DY</u>	<u>DZ</u>
214	0.0068	-0.0118	-0.0021
216	0.0071	-0.0058	-0.0035
224	-0.0031	0.0091	-0.0127
166	-0.0039	0.0101	-0.0039
173	-0.0121	-0.0169	0.0003
175	-0.0061	0.0068	-0.0100
176	0.0002	-0.0014	-0.0090
266	-0.0062	0.0077	-0.0123
273	-0.0042	0.0002	-0.0052
275	0.0156	0.0041	-0.0022
276	0.0159	-0.0045	-0.0012

The average displacement component magnitude is 0.0068 and the average radial displacement is 0.0117.

APPENDIX C OUT-OF-PLANE NEIGHBORS

Given an atom site with coordinates (0,0,0), the relative z-coordinate of each neighboring atom site changes during uniaxial compression, but the relative x- and y-coordinates do not change. If z is the relative coordinate for compression $\eta = 1.0$, then z/η is the coordinate for compression $\eta \neq 1.0$. Figures C-1 - C-11 are neighbor shell maps for the neighbors of a site marked $\square$. Neighboring sites are marked $\circ$, $\oplus$, and $\bullet$. The unit of distance is the half-lattice constant, n is the neighbor shell index, and C_n is the associated coordination number. OP means out-of-plane and IP means in-plane. The relative x- and y-coordinate of each site can be read from the map. Each nonzero relative z-coordinate is indicated as ± 1 , ± 2 , ± 3 , or ± 4 . These maps are useful in visualizing how each neighbor shell is affected by uniaxial compression.

Fig. C-1.
First neighbors.

Fig. C-2.
Second neighbors.

$n = 3$ $C_n = 24$
 $8 \text{ OP } \pm 2$
 $16 \text{ OP } \pm 1$

Fig. C-3.
 Third neighbors.

$n = 4$ $C_n = 12$
 $8 \text{ OP } \pm 2$
 4 IP

Fig. C-4.
 Fourth neighbors.

$n = 5$ $C_n = 24$
 $8 \text{ OP } \pm 3$
 $8 \text{ OP } \pm 1$
 8 IP

Fig. C-5.
 Fifth neighbors.

$n = 6$ $C_n = 8$
 $8 \text{ OP } \pm 2$

Fig. C-6.
 Sixth neighbors.

$n = 7$ $C_n = 48$
 16 OP ± 3
 16 OP ± 2
 16 OP ± 1

Fig. C-7.
Seventh neighbors.

$n = 9$ $[330]$
 $C_n = 12$
 8 OP ± 3
 4 IP

Fig. C-9.
Ninth neighbors $[330]$.

$n = 8$ $C_n = 6$
 2 OP ± 4
 4 IP

Fig. C-8.
Eighth neighbors.

$n = 9$ $[411]$
 $C_n = 24$
 8 OP ± 4
 16 OP ± 1

Fig. C-10.
Ninth neighbors $[411]$.

$n = 10$ $C_n = 24$
 8 OP ± 4
 8 OP ± 2
 8 IP

Fig. C-11.
 Tenth neighbors.