

## Calculations of Small Vacancy and Interstitial Clusters for an fcc Lattice\*

R. A. JOHNSON

Brookhaven National Laboratory, Upton, New York

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Binding and migration energies and atomic configurations have been calculated for small vacancy and interstitial clusters in an fcc lattice with a model which should be applicable to nickel. The mathematical model consisted of a spherical crystallite containing about 530 atoms which were treated as individual particles surrounded by an elastic continuum with atoms imbedded in it. A two-body central force was used to simulate the interaction between nearest-neighbor atoms in the crystallite, and the elastic continuum provided a pressure which held the crystallite in equilibrium. The binding and migration energies for divacancies and di-interstitials were  $E_{2V}^B=0.25$ ,  $E_{2V}^M=0.90$ ,  $E_{2I}^B=1.16$ , and  $E_{2I}^M=0.29$  eV. The binding energy of larger vacancy clusters was approximately equal to the energy in the nearest-neighbor "bonds" between vacancies, each "bond" contributing 0.25 eV. The vacancy-cluster migration energy increased slowly with the size of the cluster but was still less than the single-vacancy migration energy,  $E_{1V}^M=1.32$  eV, for small clusters. Spherical vacancy clusters were the most stable, although an estimate was made that a platelet on a {111} plane would collapse into a dislocation loop after absorbing somewhat more than 180 vacancies and that this loop might be more stable than a spherical cluster which had absorbed the same number of vacancies. Interstitial clustering was more complex, but in general binding energies were large and migration energies increased with cluster size, although they never got as large as that for the divacancy, the most easily migrating vacancy complex.

### I. INTRODUCTION

THE study of point defects in metals is based primarily upon the analysis of the physically measurable changes brought about by migration of the defects. Whenever an unstable number of interstitials or vacancies are present in a crystal lattice at a temperature at which they are mobile, they will encounter other such defects during their wandering as the system proceeds to a state of equilibrium. The way in which they interact has a strong effect upon the kinetics of their migration and the nature of the stable or metastable configuration to which the process eventually leads. In order that the physical changes be large enough to be measurable, experiments generally require a sufficient density of defects so that such encounters are quite common, and thus the analysis of the experiments must be based not only on the migration characteristics of the point defects themselves, but also on the way in which they interact. A recent review of annealing theory including the effect of interactions has been given by Damask and Dienes.<sup>1</sup>

Damask and Dienes<sup>2</sup> also review theoretical calculations that have been carried out pertaining to the stability and migration of small defect clusters. Such calculations are based on mathematical models of the crystal lattice which treat the lattice atomically and for which the energy change of the lattice resulting from the introduction of interstitials or vacancies can be determined. All these calculations have been carried out

for an fcc lattice and in general the parameters in the interatomic interactions have been chosen to represent copper. A number of calculations<sup>3-7</sup> for small vacancy clusters based on a Morse-function interatomic interaction have been carried out as well as several<sup>8,9</sup> which try to account for the behavior of the electrons near the defect in a more detailed way. Also, Vineyard and co-workers<sup>10</sup> and Johnson<sup>11,12</sup> and Brown<sup>11</sup> have investigated small vacancy clusters and di-interstitials using a Born-Mayer interatomic interaction. The models used in all of these calculations are open to the objection that they do not lead to an over-all interpretation of point defects and small clusters which is consistent with experimental results.

Lattice calculations for interstitials, vacancies, and close Frenkel pairs in an fcc lattice have recently been reported<sup>13</sup> which use a model applicable to nickel and which yield results consistent with the experimental data for nickel. Similar calculations have now been carried out for small clusters of interstitials and vacancies and the results are reported in the present paper.

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<sup>4</sup> A. C. Damask, G. J. Dienes, and V. G. Weizer, *Phys. Rev.* **113**, 781 (1959).

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<sup>7</sup> M. Doyama and R. M. J. Cotterill, *Phys. Rev.* **137**, A994 (1965); M. Doyama and R. M. J. Cotterill, in *Lattice Defects and their Interactions*, edited by R. R. Hasiguti (Gordon and Breach Science Publishers, Inc., New York, to be published.)

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<sup>10</sup> J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, *Phys. Rev.* **120**, 1229 (1960); G. H. Vineyard, *Discussions Faraday Soc.* **31**, 7 (1961); G. H. Vineyard, *J. Phys. Soc. Japan* **18**, Suppl. III, 144 (1963).

<sup>11</sup> R. A. Johnson and E. Brown, *Phys. Rev.* **127**, 446 (1962).

<sup>12</sup> R. A. Johnson, *J. Phys. Chem. Solids* **26**, 75 (1965).

<sup>13</sup> R. A. Johnson, *Phys. Rev.* **145**, 423 (1966).

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<sup>1</sup> A. C. Damask and G. J. Dienes, *Point Defects in Metals* (Gordon and Breach Science Publishers, Inc., New York, 1963), Chap. 2.

<sup>2</sup> A. C. Damask and G. J. Dienes, *Point Defects in Metals* (Gordon and Breach Science Publishers, Inc., New York, 1963), pp. 16-21, 37-41.

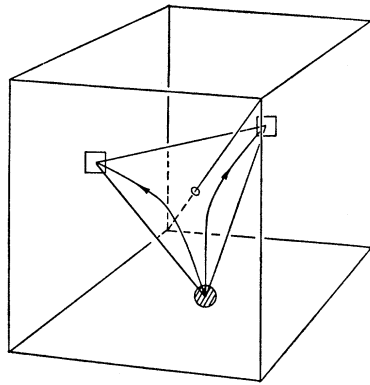


FIG. 1. The divacancy migration path. The squares represent vacancies and the shaded circle represents the jumping atom. The curved lines indicate the two possible migration paths and lie above the triangle in the plane defined by the divacancy and the jumping atom.

## II. MODEL

The model which was used for the present calculations has previously been described in detail<sup>13</sup> and only a summary will be given here. Each atom within a spherical crystallite containing about 530 atoms was treated as an independent particle with three degrees of freedom. The atoms outside this set were treated as though they were imbedded in an infinite elastic continuum and the displacement field  $\mathbf{u}$  for the elastic continuum was taken as

$$\mathbf{u} = K(\mathbf{r}/r^3).$$

The variable  $K$ , the so-called "strength" of the displacement field, was used as the only variable determining the displacement of all atoms outside the crystallite. With such a model the volume expansion associated with a lattice configuration, including a correction arising from the use of finite boundary conditions, can be shown to be linear in  $K$ .

A nearest-neighbor central interatomic interaction, which has previously been discussed in detail,<sup>13,14</sup> was used between pairs of atoms in the present calculation. The analytic form of this potential energy curve is that of three smoothly joined cubic equations for which the numerical values are given in Table I. Although this interaction was originally devised to simulate the interaction between the atoms in  $\alpha$ -iron, a bcc structure, it should be reasonably appropriate for describing the interatomic interaction in  $\gamma$ -iron or nickel, both fcc metals. The intent of the point-defect calculations for an fcc lattice was originally to investigate the nature of the physical predictions from this form of potential, but the model fits nickel sufficiently well that at most minor adjustments to the results would have to be made if an interaction specifically designed for nickel was used.

TABLE I. Interatomic interaction.

| Range (Å) | Potential (eV)                                   |
|-----------|--------------------------------------------------|
| <2.40     | $-2.195976(r-3.097910)^3 + 2.704060r - 7.436448$ |
| 2.40-3.00 | $-0.639230(r-3.115829)^3 + 0.477871r - 1.581570$ |
| 3.00-3.44 | $-1.115035(r-3.066403)^3 + 0.466892r - 1.547967$ |

<sup>14</sup> R. A. Johnson, Phys. Rev. 134, A1329 (1964).

The difference in energy between a perfect lattice and a defect lattice was found from the change in bond energy within the crystallite plus a term linear in the volume change which accounts for work done in expanding or contracting the crystallite against the pressure in the elastic continuum plus a term quadratic in the volume change which accounts for the energy stored within the elastic field. Minima, maxima, and saddle points in this energy difference were found as a function of the coordinates of all the atoms in the crystallite and the elastic strength variable  $K$  with the use of a digital computer.

## III. RESULTS

### A. Vacancies

The single-vacancy results, as reported previously,<sup>13</sup> are: vacancy formation energy  $E_{1V}^F = 1.49$  eV, formation volume  $V_{1V}^F = 0.85\Omega$ , where  $\Omega$  is the atomic volume, activation energy for migration  $E_{1V}^M = 1.32$  eV, and activation volume for migration  $V_{1V}^M = -0.05\Omega$ . Therefore, the activation energy for self-diffusion is  $E^{SD} = 2.81$  eV and the activation volume for self-diffusion is  $V^{SD} = 0.80\Omega$ . The stable vacancy configuration was that in which an atom is missing from a normal lattice site and the saddle-point configuration for migration was found by moving one of the 12 nearest-neighbor atoms to the vacancy directly towards the vacancy until it is midway between its site and the vacancy site.

The stable divacancy had a binding energy  $E_{2V}^B = 0.25$  eV, a binding volume  $V_{2V}^B = 0.02\Omega$ , and was simply the configuration in which atoms are missing from two adjacent lattice sites. The binding energy comes primarily from "bond counting," i.e., 24 bonds must be broken to create two isolated vacancies, whereas only 23 bonds must be broken to create a divacancy with the above configuration. Since short-range forces between the atoms are used in the present calculation, any more separated pair of vacancies has no bond contribution to the binding energy. The stress field contributes a negligible amount to the binding energy—never more than a few thousandths of an electron volt and usually negative—so that two vacancies separated by a lattice constant or greater distance essentially do not see each other. The binding volume associated with the divacancy is too small to be physically important.

The divacancy migration process is somewhat complicated in that the moving atom does not follow a path with very much symmetry. The activation energy for migration is  $E_{2V}^M = 0.90$  eV and the activation volume for migration is  $V_{2V}^M = -0.41$ . The migration mechanism is shown in Fig. 1, where the squares represent vacancies and the shaded circle represents the jumping atom. The curved lines indicate the two possible migration paths and lie above the triangle in the plane defined by the divacancy and the jumping atom.

In a manner similar to that for the divacancy, the binding energy of small vacancy clusters depends pri-

marily on "bond counting," i.e., the binding energy is roughly equal to the decrease in the number of broken bonds in the cluster relative to separated vacancies times the bond energy 0.25 eV. This decrease in number of broken bonds is equivalent to the number of nearest-neighbor distances between the vacancies in the cluster, and therefore the clustering can be thought of as caused by a nearest-neighbor binding energy of 0.25 eV between the vacancies. This essentially means that the most compact clusters will be the most stable. The most stable trivacancy had a binding energy of 0.76 eV and consisted of vacancies in an equilateral triangle of 3 nearest-neighbor lattice sites (3 nearest-neighbor bonds). The most stable tetravacancy had a binding energy of 1.51 eV and consisted of vacancies in a tetrahedron of 4 nearest-neighbor lattice sites (6 nearest-neighbor bonds). Results followed this pattern for higher clusters. The numerical results are summarized in Table II.

Care must be exercised to ensure that no configurations exist with a higher binding energy than those listed above for which the configuration is not simply composed of a number of atoms missing from their normal lattice sites. One such possibility for the trivacancy consists of the tetravacancy with an atom in the middle of the tetrahedron. This configuration had a binding energy of 0.59 eV and was second only to the equilateral triangle in order of stability for the trivacancies. No complicated vacancy cluster was found to seriously compete with the more simple types considered above for larger clusters.

Even though the present computer program was not designed to investigate large vacancy clusters, some conclusions relating to the collapse of clusters into dislocation loops can be made. A number of calculations were carried out to study vacancy clustering in a {111} plane. The atoms on either side of the plane tended to bow in and when clusters of up to 30 vacancies were considered, it was found that the separation of the atoms across the vacancy platelet decreased linearly with the square root of the number of vacancies in the plane, i.e., with the diameter of the vacancy platelet. With the nickel-nickel potential used in the present study, this line could be extrapolated to where the atoms would start interacting strongly across the platelet and it was found that this would occur for a platelet containing about 180 vacancies. Thus the platelet will lose its identity as a vacancy cluster after absorbing more vacancies and will be in the form of a dislocation loop. Since there is appreciable energy regained as the center of the platelet transforms into a stacking fault, the dislocation loop might become energetically more favorable than a spherical cluster. The energy barrier for collapse of a tightly packed cluster to a dislocation loop was not investigated.

The migration energy of trivacancies and higher clusters was not investigated in as great detail as for divacancies but enough calculations were carried out to determine the pattern for cluster migration. In effect, all clusters move with a higher migration energy

than divacancies. The energy for a given step in the cluster migration process is roughly the divacancy migration energy plus one-half the difference in binding energy of the initial and final configurations for the step. Since all cluster migration requires partial dissociation, all will have a higher migration energy than the divacancy. The trivacancy has an interesting feature in that it can be rearranged in any of four equivalent sites with less energy than for migration. This comes about because for each trivacancy there is only one site which completes a regular tetrahedron, and the trivacancy can flip to include any three of the tetrahedral sites by passing through the trivacancy configuration mentioned above as second to the triangle in stability, the tetravacancy with an atom at its center. To move the tetrahedron in which the trivacancy is based requires a higher energy. The trivacancy migration energy, which involves passing through a configuration with one less "vacancy bond" is about 1.02 eV, and tetravacancy migration, which involves jumping to a configuration with two less "vacancy bonds" is about 1.15 eV.

The two "rules" for vacancy clustering, (a) binding energy equal to the energy in vacancy "bonds," each bond with 0.25 eV, and (b) migration energy for a given step equal to the divacancy migration energy plus one-half the dissociation energy for the step, are considered to be sufficiently reliable and easy to apply that a general catalog of cluster results will not be given. The first was accurate to within  $\pm 0.01$  eV for clusters including up to 30 vacancies, and the second, although more approximate, should reflect the qualitative predictions of the model.

## B. Interstitials

The single-interstitial results, as reported previously,<sup>18</sup> are: interstitial formation energy  $E_{1I}^F = 4.08$  eV, formation volume  $V_{1I}^F = 0.7\Omega$ , activation energy for migra-

TABLE II. Summary of calculated results for vacancy and interstitial clusters in nickel. Energies are in eV. Superscript *F* means formation, *M* means motion, *B* means binding, and *R* means reorientation. The fractions listed with interstitial clusters are the probability that the given number of interstitials will be in the correct channels to give the particular configuration.

| Vacancies<br>(vacancy interactions<br>were short-ranged) |      | Interstitials<br>(interstitial interactions<br>were long-ranged) |                         |
|----------------------------------------------------------|------|------------------------------------------------------------------|-------------------------|
| $E_{1V}^F$                                               | 1.49 | $E_{1I}^F$                                                       | 4.08                    |
| $E_{1V}^M$                                               | 1.32 | $E_{1I}^M$                                                       | 0.15                    |
| $E_{2V}^{SD}$                                            | 2.81 | $E_{2I}^B$                                                       | 1.16                    |
| $E_{2V}^B$                                               | 0.25 | $E_{2I}^M$                                                       | 0.29 $\frac{3}{4}$      |
| $E_{2V}^M$                                               | 0.90 | $E_{2I}^R$                                                       | 0.05 $\frac{1}{4}$      |
| $E_{3V}^B$                                               | 0.76 | $E_{3I}^B$                                                       | 2.85                    |
| $E_{3V}^M$                                               | 1.02 | $E_{3I}^M$                                                       | 0.45 $\frac{3}{8}$      |
| $E_{4V}^B$                                               | 1.51 | $E_{3I}^R$                                                       | 0.15                    |
| $E_{4V}^M$                                               | 1.15 | $E_{3I}^B$                                                       | 2.37 $\frac{9}{16}$     |
|                                                          |      | $E_{3I}^R$                                                       | Negative $\frac{1}{16}$ |
|                                                          |      | $E_{4I}^B$                                                       | 4.1                     |

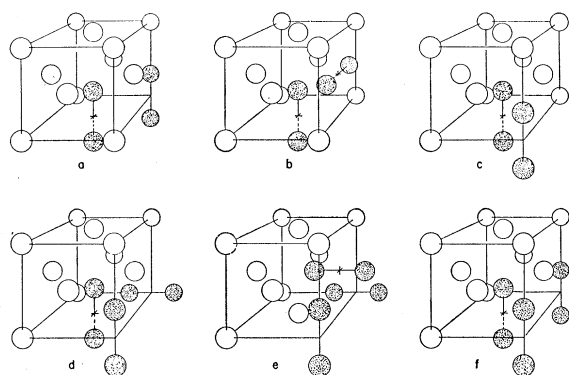


FIG. 2. Di-interstitial and tri-interstitial configurations. Figures (a) and (c) show two different but equivalent stable di-interstitials, and (b) shows a metastable configuration through which a di-interstitial passes in migration from (a) to (c). Two tri-interstitials which are energetically equivalent but which have a different orientation to their strain field are shown in (d) and (e). These are forms of the most stable tri-interstitial and the reorientation energy is lower than the migration energy. Another form of tri-interstitial is shown in (f) which cannot convert into the most stable form by elementary steps of its component interstitials. There is only a  $\frac{3}{8}$  probability that three single interstitials will be in the appropriate channels to give the most stable tri-interstitial, and  $\frac{9}{16}$  probability that it will be in the form in (f). There is a third form with  $\frac{1}{16}$  probability. The di-interstitial shown in (a) and (c) has a  $\frac{3}{4}$  probability, and there is one other di-interstitial form with a  $\frac{1}{4}$  probability.

tion  $E_{1I}^M = 0.15$  eV, and activation volume for migration  $V_{1I}^M = 0.1\Omega$ . The most stable interstitial configuration was the  $\langle 100 \rangle$  split configuration in which two atoms are symmetrically displaced in the  $\langle 100 \rangle$  direction from a vacant lattice site. The migration mechanism consisted of one end of the split jumping to form a split at a nearest-neighbor lattice site. This involves rotation of the axis of the split as well as migration. Another metastable interstitial was found which gives rise to a different migration mechanism—the  $\langle 111 \rangle$  split—in which two atoms are symmetrically displaced in the  $\langle 111 \rangle$  direction from a vacant lattice site. Again the migration mechanism consisted of one end of the split jumping to form a split at a nearest-neighbor lattice site. The configuration was metastable by  $E_{1I}^S(\langle 111 \rangle \text{ split}) = 0.16$  eV and the activation energy for migration was  $E_{1I}^M(\langle 111 \rangle \text{ split}) = 0.13$  eV. The  $\langle 110 \rangle$  split configuration, the so-called crowdion, was just barely metastable and migrated very easily:  $E_{1I}^S(\langle 110 \rangle \text{ split}) = 0.02$  eV, and  $E_{1I}^M(\langle 110 \rangle \text{ split}) = 0.04$  eV.

There are many metastable di-interstitials and unlike the vacancy case, interstitials were found to interact at appreciable separation distances. The most stable pair consisted of two parallel  $\langle 100 \rangle$  single interstitials at nearest-neighbor lattice sites with the line joining their centers perpendicular to their axes, as shown in Fig. 2(a). The binding energy was  $E_{2I}^B = 1.16$  eV. The migration energy was  $E_{2I}^M = 0.29$  eV and the migration mechanism consists of a two-step process in which, starting from the configuration in Fig. 2(a), one interstitial first jumps to form the complex shown in Fig. 2(b) and then either goes back to its original location or jumps to the configuration shown in Fig. 2(c), which is

equivalent to that in Fig. 2(a), i.e., a stable di-interstitial. This migration mechanism involves motion in a plane, and migration perpendicular to the plane requires a considerably greater activation energy. The configuration in Fig. 2(b) is metastable by 0.07 eV and was the second most tightly bound di-interstitial with a binding energy of 0.94 eV. For interstitial cluster migration, the “rule of thumb” for migration energies is that  $E^M$  equals the single interstitial migration energy plus one-half the decrease in binding energy for the step. The rule for the step given above yields 0.26 eV, whereas the carefully calculated result was 0.29 eV.

Di-interstitial calculations out to fourth-neighbor separation distances were carried out and the results indicate a very complex pattern. Even at this separation one configuration (an interstitial at the origin split in the  $x$  direction and one at  $[220]a/2$  split in the  $z$  direction, where  $a$  is the lattice constant) was bound by 0.45 eV and another (an interstitial at the origin split in the  $x$  direction and one at  $[220]a/2$  split in the  $x$  direction) was repulsive by 0.44 eV. As pointed out earlier,<sup>13</sup> there are four migration channels for interstitials and the present results shown that in general interstitials in the same channel repel one another, whereas interstitials in different channels can find an appropriate mechanism for becoming tightly bound. The most tightly bound configuration is excluded for interstitials in the same channel, but since their interaction varies with configuration, there are “trapping” configurations in which the energy to separate is greater than the normal interstitial migration energy (one such site involves an interstitial at the origin split in the  $z$  direction and one at  $[200]a/2$  split in the  $z$  direction).

In summary, three-fourths of possible interstitial encounters proceed in a normal way with a long-range attractive interaction to a tightly bound complex which migrates with a higher energy than a single interstitial. The other fourth of possible encounters produces a complex pattern within which the interstitials will never become tightly bound, in general repel each other, but can trap each other, or in effect be loosely bound.

The results from the study of tri-interstitials are even more complicated. The basic features that emerge are a very tightly bound defect,  $E_{3I}^B = 2.85$  eV, a migration energy higher than that of di-interstitial,  $E_{3I}^M \approx 0.45$  eV, and a reorientation mechanism which could, for example, give rise to stress-induced ordering with an energy about the same as that for the single-interstitial migrating energy,  $E_{3I}^R \approx 0.15$  eV. The most stable configuration involves an atom at  $[110]a/2$  with an  $x$  orientation, an atom at  $[000]$  with a  $z$  orientation, and an atom at  $[1\bar{1}0]a/2$  with a  $z$  orientation as shown in Fig. 2(d). An equivalent configuration with a different orientation is shown in Fig. 2(e). Because of the existence of separate channels for the split interstitials, there is only a  $\frac{3}{8}$  probability that three interstitials can form the most stable tri-interstitial. The probability is  $\frac{9}{16}$  that their most stable configuration will be bound by 2.37 eV and involves an atom at  $[110]a/2$ , an atom at

[000], and an atom at  $[\bar{1}\bar{1}0]a/2$ , all with  $z$  orientations as shown in Fig. 2(f). Although this configuration has a strong orientation dependence, there is no mechanism for reorientation and thus it cannot give rise to an ordering effect. In the more tightly bound configuration, none of the interstitials are in the same migration channel, whereas in this case, two interstitials are in the same channel. There is a  $\frac{1}{16}$  probability that they will all be in the same channel, but these configurations give very little binding and are analogous to the di-interstitial cases in which both interstitials are in the same channel.

Several tetra-interstitial configurations were run and binding energies were in the range of 4.1 eV. Since the interaction between interstitials is very complex, simple patterns in the binding energy such as were found for vacancy clusters are not seen for interstitial clusters.

In all the above interstitial clusters it was assumed that the component interstitials were of the  $\langle 100 \rangle$  split type. Several trials were made to find di-interstitial configurations based on  $\langle 111 \rangle$  split or  $\langle 110 \rangle$  split interstitials, and although some very tightly bound configurations were found, they all tended to decay quite easily to the most stable form discussed above.

In summary, interstitial clusters did not show a clear pattern in configuration or binding energy. Clusters are tightly bound and the migration energy increases with size of the cluster. The numerical results are listed in Table II.

#### IV. DISCUSSION

Damask and Dienes<sup>2</sup> review early estimates of divacancy binding energies and trivacancy stability for copper. These calculations in general give results in the range of 0.3–0.6 eV for divacancy binding energies and indicate that the trivacancy consisting of an extra atom centered in a tetrahedron of vacancies is more stable than a nearest-neighbor triangle. The present results will be compared to results using a Born-Mayer interaction<sup>10–12</sup> and to some recent calculations using a Morse interaction.<sup>7</sup> These two sets of results are the most detailed and the most representative of the given interaction.

The Born-Mayer interaction gives rise to a two-body central repulsion between nearest neighbors, and very little interaction for more distant neighbors. Thus neighboring atoms to a vacancy can relax slightly inward towards a vacancy, but there is little energy change during the relaxation process. The bond-counting contribution is also small, and in this case negative. For divacancy binding the additional relaxation caused by the proximity of another vacancy is slightly greater than the bond-counting contribution, and so there is a net small binding energy: 0.06 eV. The same trend is observed, e.g., for a trivacancy in which the vacant sites are in a  $\langle 110 \rangle$  tight-packed line—here the binding energy is negative,  $-0.1$  eV. Vacancy cluster configurations which permit atoms to get further away from their neighbors by a large relaxation

are much more favored, however; for example, the trivacancy consisting of a tetravacancy with an atom in the middle has a binding energy of 0.46 eV. This trend also continues for larger clusters. Thus the configurations and to some degree also the energies are strikingly different than those found in the present report. The same is true for divacancy migration, where the Born-Mayer interaction gives a very small value: 0.07 eV, whereas the value reported in the present work is 0.90 eV. The Born-Mayer models are intended to simulate copper, whereas the present report should be applicable to nickel; but this should not be important since the radiation-damage annealing patterns in the two metals are similar, and also since a Born-Mayer calculation for nickel would give results similar to the Born-Mayer copper results, and a copper calculation using the present form of potential would give results similar to those reported for nickel.

There were not many Born-Mayer calculations made for interstitial clusters, but the interstitial results are in better agreement since the binding does not explicitly come from the interaction, but arises primarily from reinforcement of the strain fields from each of the interstitials. The same di-interstitial was found to be stable and the same interstitial and di-interstitial migration mechanisms were found, although the present work gives binding and migration energies somewhat higher than the Born-Mayer results. These values for nickel should be somewhat higher than for copper.

The calculations based on a Morse interaction<sup>7</sup> present yet another picture. They yield a tightly bound divacancy,  $E_{2V}^B = 0.53$  eV, but also give a small divacancy migration energy,  $E_{2V}^M = 0.03$  eV. The vacancy cluster configurations indicate a different pattern and were reported to be tightly bound. The trivacancy consisting of three nearest-neighbor vacancies (the same one found to be most stable in the present report) was reported as being the most stable with a binding energy  $E_{3V}^B = 2.23$  eV. But the most stable tetravacancy was found to consist of the above triangular trivacancy plus a nearest-neighbor vacancy to two of those in the triangle, which means it is in the plane defined by the triangle. Thus the authors believe the model, if run for larger clusters, would favor vacancy platelets in the  $\{111\}$  plane right from the smallest size. Interstitial clusters were not calculated.

These comparisons are summarized in Table III, and the rather extreme differences in the three models are easily seen. Again remembering that the Born-Mayer and Morse calculations are for copper and the present for nickel, some of the predictions of these models can be compared with experimental values. Using the data in two recent review papers,<sup>15,16</sup> one finds that the values for single-vacancy migration in copper range from 0.88

<sup>15</sup> J. W. Corbett, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1966), Suppl. 7.

<sup>16</sup> A. Seeger and D. Schumacher, in *Lattice Defects in Quenched Metals*, edited by R. M. J. Cotterill, M. Doyama, J. J. Jackson, and M. Meshii (Academic Press Inc., New York, 1965), p. 15.

TABLE III. Comparison of the clustering characteristics from different models. Energies are in eV.

|                  | Born-Mayer <sup>a</sup> | Morse <sup>b</sup>   | Present              |
|------------------|-------------------------|----------------------|----------------------|
| $E_{1V}^M$       | 0.43                    | 0.69                 | 1.32                 |
| $E_{2V}^B$       | 0.06                    | 0.53                 | 0.25                 |
| $E_{2V}^M$       | 0.07                    | 0.03                 | 0.90                 |
| $E_{3V}^B$       | 0.46                    | 2.23                 | 0.76                 |
| 3V configuration | filled tetrahedron      | equilateral triangle | equilateral triangle |
| $E_{4V}^B$       | 0.7                     | 3.85                 | 1.51                 |
| 4V configuration | complex                 | {111}                | tetrahedron          |
| $E_{1I}^M$       | 0.05                    | 0.15                 | 0.15                 |
| $E_{2I}^B$       | 0.61                    |                      | 1.16                 |
| $E_{2I}^M$       | 0.08                    |                      | 0.29                 |

<sup>a</sup> See Refs. 10-12.<sup>b</sup> See Ref. 7.

to 1.08 eV and in nickel from 1.35 to 1.55 eV. Thus the nickel calculations agree better, but not strikingly so. The copper divacancy binding and migration energies are thought to be about 0.1 and 0.6 eV, respectively, while the nickel divacancy migration energy is in the range of 0.8-1.0 eV. Especially with regard to the divacancy migration energy, the Born-Mayer and Morse

results are in conflict with the data, whereas the present calculations are in agreement. The single-interstitial results were discussed previously,<sup>13</sup> and no reliable interstitial-clustering data are available.

The primary difference between the present calculations and those using either Born-Mayer or Morse interactions is that the interaction used here gives rise to a nearest-neighbor "bond" which must be broken if the atoms are to be separated at all. The Born-Mayer interaction is purely repulsive and the Morse, although it has an attractive tail binding atoms together, is long in range, so that motions of the order of a nearest-neighbor distance do not involve making or breaking the "bond" between atoms. It is the existence of this bond which gives rise to reasonable values of vacancy and divacancy migration energies in the present calculations.

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## Dislocation Velocities in a Two-Dimensional Model\*

W. F. HARTL† AND J. H. WEINER

Department of Mechanical Engineering, Columbia University, New York, New York

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The dynamics of an edge dislocation in a two-dimensional crystal model are investigated using a localized unstable normal mode of vibration of the model. The model used is a simple-cubic lattice with linear central and noncentral nearest-neighbor interactions and a piecewise linear restoring force between atoms on the slip plane. The atoms below the slip plane are fixed. Lattice parameters are chosen to allow specific stable and unstable configurations of the lattice, and it is assumed that the dislocation progresses by passing alternately through stable and unstable states. It is found that there is one localized unstable mode of vibration whose components are very large in the neighborhood of the dislocation. This localized mode is used to approximate dislocation motion in the unstable state, and it is altered—by symmetrizing it with respect to the stable lattice configuration—to approximate motion in the stable state. Two coordinates, given by harmonic equations of motion, then characterize the dynamics of the dislocation. The relation between the two coordinates gives an energy-loss mechanism which leads to a steady-state dislocation velocity when a shear stress is applied to the lattice. Transient and steady-state velocities and the minimum stress necessary to maintain a steady-state velocity are calculated. The same quantities are found using computer simulation of a finite lattice, and a comparison is made. Reasonably good agreement is found for velocities up to about 0.7 times the velocity of sound in the continuum in the direction of slip. The analytic theory underestimates the minimum stress necessary to maintain a steady-state velocity.

### I. INTRODUCTION

IN spite of the importance of the subject, little theoretical work has been done on the dynamics of dislocations in crystals from a discrete, microscopic

viewpoint. The earliest work on two-dimensional dislocation dynamics considered a single volterra dislocation in an infinite elastic continuum; in this model the dislocation may move freely at any velocity less than the speed of sound without an applied stress.<sup>1</sup> A similar solution was found<sup>2,3</sup> for a modified continuum

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† Currently NAS-NRC Postdoctoral Fellow at Institute for Materials Research, National Bureau of Standards, Washington, D. C.

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