Energy and Atomic Configurations of Complete and Dissociated Dislocations. II. Screw Dislocation in an fcc Metal*

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The arrangement of atoms around a screw dislocation in copper has been calculated by a variational method. The pairwise interaction between discrete atoms was represented by a Morse potential function. The displacements parallel to the dislocation line agree well with those given by linear elastic theory except for atoms within a distance of about 5.3 Å of the center of the dislocation. Because of this, there is a disparity between the atomistic and elastic energies inside a core radius of 5.3 Å for a complete ⟨110⟩ screw dislocation (Burgers vector $=(a_0/2)\langle 110\rangle$), where a_0 is the lattice parameter. The corresponding core energy is 1.0 eV per nearest-neighbor distance. In the calculation of the complete dislocation, the atoms were not permitted to relax in a direction perpendicular to the dislocation line. This prevented dissociation. When this constraint is removed, dissociation into two partial dislocations occurs spontaneously. If the core is replaced by a hole of radius r_{eh} (the *equivalent hole radius*), the inside of which is hollow and outside of which linear-elastic theory holds at all points, this radius is 1.1 Å. The energy of the screw dislocation varies as $\ln r$ at large radii, in agreement with elastic-continuum theory. By comparing this asymptotic behavior with the corresponding curve for the edge dislocation, atomistic values of the shear modulus and Poisson's ratio were obtained.

I. INTRODUCTION

In a previous paper[1] (hereafter referred to as Paper I), it was shown that the difficulties associated with the core of an edge dislocation can be successfully overcome by the use of an atomistic model. Such a model was used in a computer calculation of the positions of the atoms in the core of an edge dislocation, and the core radius and core energy were computed for a ⟨112⟩ dislocation (Burgers vector $(a_0/2)\langle 110\rangle$, where a_0 is the lattice parameter). The relaxed positions of the atoms in the dislocation were compared with the positions given by elastic theory and certain important discrepancies were noted. In particular, the displacements parallel to the dislocation line were found to be finite and to have both positive and negative sign. The isotropic elastic theory predicts that these displacements should be zero. These nonzero displacements indicated that the dislocation was dissociating. They were artificially held at zero to prevent this dissociation and hence permit a calculation of the core energy and atomic configuration of a complete dislocation.

This paper describes a similar investigation of the atomistic properties of a screw dislocation in an fcc metal. Such a calculation affords a comparison between edge and screw dislocations on an atomic scale.

Not all of the rough estimates of the core energy cited in Paper I distinguish between the cores of edge and screw dislocations. Bragg's estimate,[2] for instance, which used the fact that the energy density in the core cannot exceed the latent heat of melting, appears to be applicable to both types of dislocation. The estimate was 1 eV per atom plane. Hasiguti and Doyama[3] used the fact that if two parallel screw dislocations having opposite signs are separated by one atomic layer the long-range stress fields cancel and all the interaction energy is stored in the dislocation cores. They calculated the interaction energy by assuming that elastic theory holds down to atomic distances and obtained a core energy of under 1.0 eV per atom plane. Cottrell's estimate,[4] based on the assumption that Hooke's law holds inside the core, gives 1.3 eV per atom plane for an edge dislocation. If the same assumption holds for a screw dislocation and if the core size is the same for both types of dislocation, the core energy should be $(1-\nu)$ times the core energy of an edge dislocation, where ν is Poisson's ratio. Taking ν to be $\frac{1}{3}$ in a typical face-centered cubic metal, we find that the core energy of a screw dislocation should be about 0.8 eV per atom plane. Huntington *et al.*[5] have investigated the core of a screw dislocation in sodium chloride.

The present investigation was carried out with the aid of a CDC 3600 digital computer. The pairwise interaction between atoms was represented by a truncated Morse potential function.

II. NATURE OF THE PROBLEM

When calculated by the isotropic elastic-continuum theory, the displacements parallel to the three axes x, y, and z, due to a screw dislocation lying along the x axis, are, respectively,

$$u=\frac{b}{2\pi}\arctan\frac{z}{y}, \qquad v=0, \qquad w=0, \tag{1}$$

* Based on work performed under the auspices of the U. S. Atomic Energy Commission.

[1] R. M. J. Cotterill and M. Doyama, Phys. Rev. **145**, 465 (1966).

[2] W. L. Bragg, *Symposium on Internal Stress* (Institute of Metals, London, 1947), p. 221.

[3] R. R. Hasiguti and M. Doyama, Bull. Japan Inst. Metals, October (1952) [in Japanese]; Bull. Phys. Soc. Japan, April (1953).

[4] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Clarendon Press, Oxford, 1953), p. 39.

[5] H. B. Huntington, Phys. Rev. **59**, A942 (1941). H. B. Huntington, J. E. Dickey, and R. Thomson, *ibid.* **100**, 1117 (1955).

where b is the Burgers vector. For a sufficiently large crystal the elastic energy per unit length of the dislocation is

$$E^s=\frac{\mu b^2}{4\pi}\left[\ln\left(\frac{r_1}{r_c{}^s}\right)-1\right]+E_{\text{core}}{}^s, \tag{2}$$

where μ is the shear modulus, $r_c{}^s$ is the core radius, $E_{\text{core}}{}^s$ is the core energy, and r_1 is the outer radius of the crystal. In all cases the superscript letter s denotes applicability to the screw dislocation. The second term in the brackets arises from relaxation of surface stresses.

The energy per unit length of a cylinder of radius r inside the crystal, with the dislocation along its axis, is

$$E^s(r)=\frac{\mu b^2}{4\pi}\left[\ln\left(\frac{r}{r_c{}^s}\right)-1\right]+E_{\text{core}}{}^s. \tag{3}$$

Differentiating Eq. (3) with respect to r we have

$$\frac{dE^s}{dr}=\frac{\mu b^2}{4\pi}\frac{1}{r}, \tag{4}$$

and Eq. (4) can be plotted to give the curve shown in Fig. 1. The substitution

$$E_{\text{core}}{}^s=\frac{\mu b^2}{4\pi}\left(\ln\frac{r_c{}^s}{r_{\text{eh}}{}^s}\right) \tag{5}$$

(where $r_{\text{eh}}{}^s$ is the *effective hole radius*) can be used to change Eq. (3) to

$$E^s(r)=\frac{\mu b^2}{4\pi}\ln\frac{r}{r_{\text{eh}}{}^s}, \tag{6}$$

and we see that for the screw dislocation, too, the dislocation behaves as if it had a hollow hole of radius $r_{\text{eh}}{}^s$ down its axis and that outside this hole the linear-elastic theory is obeyed at all points. The position of $r_{\text{eh}}{}^s$ is clearly such that the area lying under the dashed curve between $r_{\text{eh}}{}^s$ and $r_c{}^s$ in Fig. 1 (the vertically shaded region) is equal to the area under the solid curve between $r=0$ and $r_c{}^s$ (the horizontally shaded region).[6] As before, we expect $r_{\text{eh}}{}^s$ to be somewhat smaller than $r_c{}^s$, the core radius.

It is worth noting that Eq. (6) and its counterpart for the edge dislocation (where the superscript letter E refers to the edge dislocation),

$$E^E(r)=\frac{\mu b^2}{4\pi(1-\nu)}\ln\frac{r}{r_{\text{eh}}{}^E}, \tag{7}$$

can be combined to give

$$E^s(r)/E^E(r)=(1-\nu)[\ln(r/r_{\text{eh}}{}^s)]/[\ln(r/r_{\text{eh}}{}^E)], \tag{8}$$

[6] In reality the solid line in Fig. 1 is not continuous because the crystal is atomistic. The horizontally shaded region should therefore be replaced by a histogram having the same area.

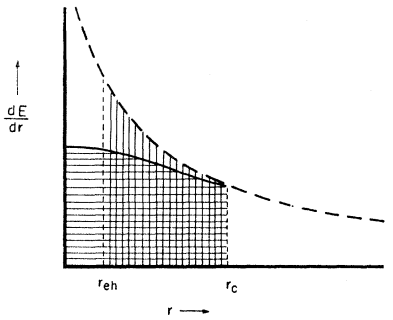

FIG. 1. Schematic plot of dE/dr as a function of r for a dislocation. r is the distance from the center of the dislocation and E is the energy within a radius r. r_c and r_{eh} are the core and equivalent hole radii, respectively. The areas of the horizontally and vertically shaded regions are both equal to the core energy.

and for large r this gives the classical result

$$E^s(r)=(1-\nu)E^E(r) \tag{9}$$

for equal lengths of edge and screw dislocations having the same Burgers vector.

III. METHOD OF COMPUTATION

A. The Crystal Model

The screw dislocation investigated here lies along a ⟨110⟩ direction. Its Burgers vector was therefore of the $(a_0/2)\langle 110\rangle$ type. There are just two nonequivalent types of plane normal to a ⟨110⟩ direction in the fcc lattice. Outside these adjacent planes the pattern is repeated. All realxing operations could therefore be carried out only on atoms in these planes, and the crystal was made effectively infinite along the dislocation line by use of periodic boundary conditions which permitted simultaneous movement of equivalent atoms. The number of atoms in each {110} plane normal to the dislocation line was about 2000.

The [110] dislocation line was along the x axis, and the y and z axes were placed along $[\bar{1}12]$ and $[1\bar{1}1]$ directions, respectively. The units along these axes were chosen so as to allow the position of each atom to be described by integer coordinates. The units along the x, y, and z axes were $d/2$, $d/2\sqrt{3}$, and $(\sqrt{\frac{2}{3}})d$, respectively, where d is the atomic spacing. The dislocation cut the yz plane at $y=0$, $z=0.5$.

Calculations of the energy and atomic configuration of the dislocation were made for both *elasto-atomic* and *atomistic* models. The atoms in the *elasto-atomic* model were treated as discrete atoms embedded in an elastic "ether." Their energies were calculated according to interactions using the Morse potential function described briefly in the next section. This model was also used as a starting point for the *atomistic* calculation in which the atoms were allowed to relax individually until equilibrium prevailed.

The positional coordinates of the atoms in the perfect crystal were first fed into the computer, and the energy

of each atom (E_0) was calculated. The crystal was then deformed in such a way that the atoms were displaced by amounts consistent with Eqs. (1). The energy of the resultant elasto-atomic screw dislocation was calculated as a function of radial distance from the center of the dislocation. The atoms were then relaxed, one at a time, until equilibrium prevailed throughout the crystal. This process required a number of relaxations of each atom, and the relaxations were carried out in cycles in which atoms near the center of the dislocation which suffer the greatest displacements were relaxed most often. The energy of the resulting atomistic dislocation was also calculated as a function of radial distance from the center of the dislocation. In the calculation of the energy and atomic arrangement of the complete screw dislocation, the atoms were not permitted to relax in a direction perpendicular to the dislocation line. When such relaxation is allowed, the dislocation spontaneously dissociates, as is discussed later. The strain energy inside a certain radius is

$$\tfrac{1}{2}\sum_{i=1}^{n}(E_i-E_0),$$

where n is the number of atoms inside that radius, E_i is the energy of the ith atom after relaxation, and the factor $\frac{1}{2}$ is required because each interatomic bond is counted twice in the summation.

B. The Morse Potential Function

In the present calculations the interaction energy between atoms was represented by a central force function. A Morse function was used because this has both attractive and replusive terms and a perfect crystal which obeys this function can be made stable even without the application of surface forces. The interaction energy $E(r_{ij})$ of a pair of isolated atoms is then given by

$$E(r_{ij})=D\{\exp[-2\alpha(r_{ij}-r_0)] -2\exp[-\alpha(r_{ij}-r_0)]\}, \quad (10)$$

where r_{ij} is the distance between the two atoms, D is the dissociation energy of the pair, r_0 is the equilibrium separation distance of the two atoms, and α is a constant which is effectively a measure of the "hardness" of the interaction. The energy of any atom in the crystal is then E_i, where

$$E_i=\sum_{j=1}^{j=J}E(r_{ij}), \quad (11)$$

and where J is the number of atoms in the sphere of influence. J is, of course, related by a geometrical factor to the distance over which the interaction extends. Girifalco and Wiezer[7] have derived constants for the Morse potential for several different metals. For copper these authors give $\alpha=1.3588$ Å^{-1}, $r_0=2.8660$ Å, and $D=0.34290$ eV.

The values of the constants must, of course, depend upon J. Clearly, if J were 12 (i.e., only nearest-neighbors interact), then r_0 would be equal to the nearest-neighbor distance. The values given by Girifalco

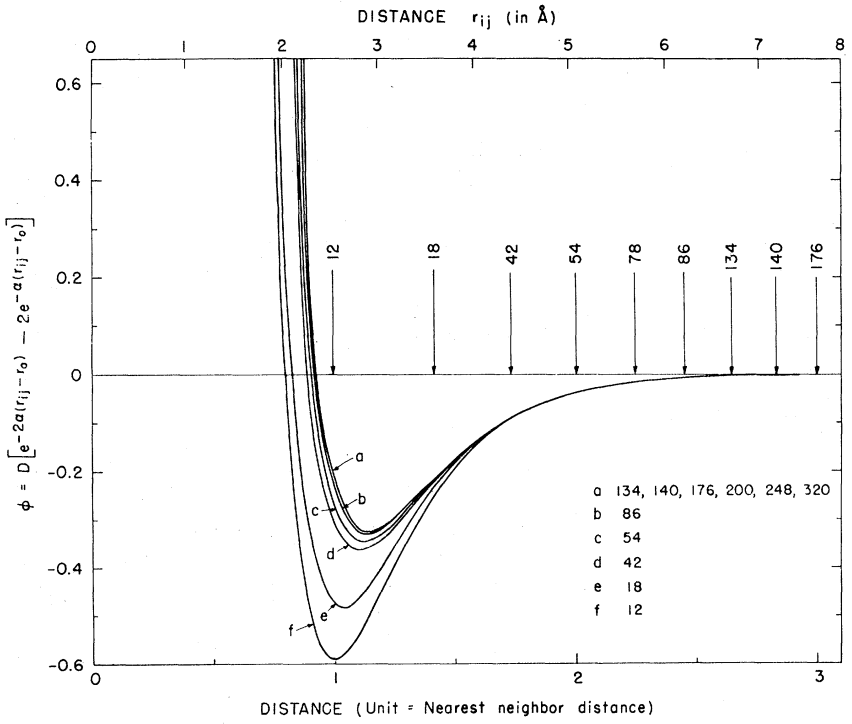

FIG. 2. The Morse potential for copper plotted as a function of distance for various truncations. The constants of the potential were derived from the sublimation energy.

[7] L. A. Girifalco and V. G. Weizer, Phys. Rev. 114, 687 (1959).

and Wiezer were obtained with a large crystal (containing 4000 atoms) in which each atom was allowed to interact with all other atoms. The field of each atom therefore virtually extended to infinity. In variational calculations of the type used here, the successive relaxations of atoms are rather time consuming even when the latest computers are employed; so it becomes impracticable to consider such long-range interactions. Moreover, one cannot be certain that the field of an atom is still adequately described by a Morse function at distances greater than a few nearest-neighbor distances. One would expect screening effects from other atoms to modify the field. For both of these reasons it becomes desirable to truncate the potential (i.e., to limit J to some convenient finite number). It can be shown[8] that as J decreases from infinity to 12 (the number of nearest-neighbor atoms in the perfect fcc lattice), the value of r_0 decreases from about $1.3d_0$ to d_0, where d_0 is the nearest-neighbor distance. There is also a corresponding variation in α and D. In the work described here the potential was truncated at 176 neighboring atoms and the constants were $r_0=2.9130$ Å, $a_0=3.6028$ Å, $D=0.3227$ eV, and $\alpha=1.2866$ Å^{-1}, where a_0 is the lattice constant ($=d_0\sqrt{2}$). These constants were determined by the method described by Girifalco and Wiezer.[7] The Morse potential for these constants is plotted as a function of truncation in Fig. 2. Although the different curves in Fig. 2 refer to different truncations they have all been extended out to the asymptotic limit. This is necessary because, even though the truncation may eliminate all but a few of the neighboring atoms, some of the latter may nevertheless be displaced to relatively large distances when the lattice is under strain. This method uses the fact that bulk crystal properties calculated with a particular truncated potential must match the experimental values of those properties. In this case the properties chosen were the energy of sublimation, the bulk modulus, and the lattice constant. An additional constraint was that the Born stability criteria have to be satisfied. Moreover, the potential used here gives values of the elastic constants which are in good agreement with the experimental values. The experimental values of C_{11}, C_{12}, and C_{44} are 17.88×10^{11} dyn cm^{-2}, 12.6×10^{11} dyn cm^{-2}, and 8.25×10^{11} dyn cm^{-1}, respectively.[9] The theoretical values derived with the Morse potential were 15.98×10^{11} dyn cm^{-2}, 11.22×10^{21} dyn cm^{-2}, and 11.22×10^{11} dyn cm^{-2} for the same quantities. In deriving these elastic constants the Cauchy relation has to be obeyed because only central forces are considered. Thus the theoretical values of C_{12} and C_{44} are always equal. Because of this an effective value of C_{12}, which was simply the mean of the experimental values of C_{12} and C_{44}, was used to calculate an effective bulk modulus. This procedure afforded the best compromise agreement between the experimental and theoretical values of C_{11}, C_{12}, and C_{44}. This procedure was also adopted in the work described in Paper I. The value of E_0 was -7.07066 eV.

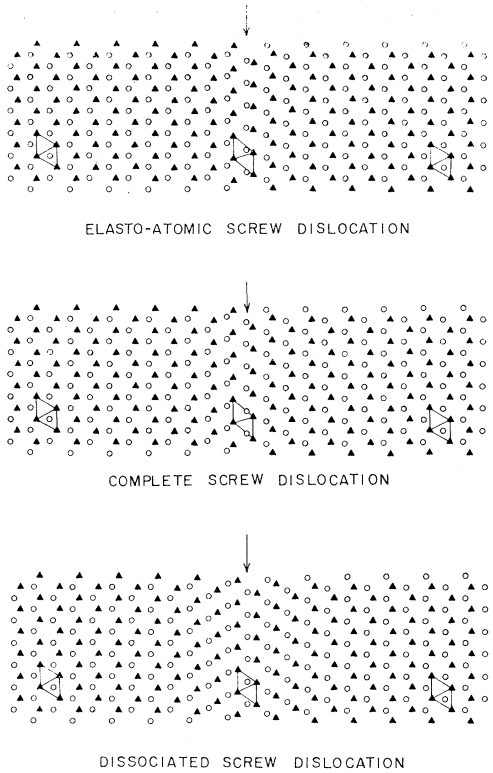

FIG. 3. Positions of atoms in two {111} planes, one above (triangles) and one below (circles) the slip plane of a screw dislocation. The dislocation line lies along the ⟨110⟩ direction indicated by the arrow. A narrow region of stacking fault lies at the center.

IV. RESULTS

A. Complete Screw Dislocation

For calculations on the complete screw dislocation, the atoms were not permitted to relax in any direction perpendicular to the dislocation line. This prevented dissociation. The positions of the atoms near the center of the dislocation, and in (111) planes immediately above and below the slip plane, are plotted in Fig. 3(b). For the sake of comparison the corresponding positions of atoms in the elasto-atomic approximation are given in Fig. 3(a). The positions of some of the atoms near the center of the dislocation for both the elasto-atomic and atomistic cases of the complete screw dislocation are given in Tables I and II. Also given is the energy E_i of each atom.

The energy of the complete screw dislocation is plotted as a function of radius in Fig. 4. Again, both the elasto-atomic and atomistic energies are plotted. The energies are plotted against $\ln r$ so that the extent

[8] M. Doyama and R. M. J. Cotterill, Bull. Am. Phys. Soc. 10, 323 (1965).

[9] H. B. Huntington, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Vol. 7, p. 213.

TABLE I. Positions and energies of atoms around elasto-atomic screw dislocation.

Identity			Coordinates x	y	z	Distance from the center in nearest-neighbor distances (Å)	Energy E_i (eV)
0	0	0	−0.500	0.000	0.000	0.408	−6.550
−1	1	1	−0.696	1.000	1.000	0.500	−6.511
0	−2	1	0.804	−2.000	1.000	0.707	−6.789
1	3	0	0.860	3.000	0.000	0.957	−6.889
1	−3	0	0.140	−3.000	0.000	0.957	−6.867
0	4	1	0.108	4.000	1.000	1.224	−6.983
1	−1	−1	0.426	−1.000	−1.000	1.258	−7.016
1	−1	2	1.574	−1.000	2.000	1.258	−6.958
0	2	−1	−0.360	2.000	−1.000	1.354	−6.953
0	2	2	0.360	2.000	2.000	1.354	−7.026
−1	−5	1	−0.088	−5.000	1.000	1.500	−7.014
0	−4	2	0.741	−4.000	2.000	1.683	−6.991
0	−4	−1	−0.741	−4.000	−1.000	1.683	−7.031
0	−6	0	−0.926	−6.000	0.000	1.780	−7.039
0	6	0	−0.074	6.000	0.000	1.780	−7.029
1	5	−1	0.776	5.000	−1.000	1.893	−7.011
1	5	2	1.224	5.000	2.000	1.893	−7.040
0	0	3	0.500	0.000	3.000	2.041	−7.032
−1	7	1	−0.937	7.000	1.000	2.062	−7.046
−1	1	−2	−1.455	1.000	−2.000	2.062	−7.027
0	−2	−2	−0.588	−2.000	−2.000	2.121	−7.043
1	−3	3	1.628	−3.000	3.000	2.217	−7.026
1	3	3	1.372	3.000	3.000	2.217	−7.047
0	−8	1	0.944	−8.000	1.000	2.345	−7.044
0	4	−2	−0.336	4.000	−2.000	2.345	−7.029
1	−7	2	1.827	−7.000	2.000	2.363	−7.036
1	−7	−1	0.173	−7.000	−1.000	2.363	−7.052
−1	−5	−2	−1.696	−5.000	−2.000	2.500	−7.052
0	8	2	0.155	8.000	2.000	2.614	−7.054
0	8	−1	−0.155	8.000	−1.000	2.614	−7.042
1	9	0	0.950	9.000	0.000	2.630	−7.048
1	−9	0	0.050	−9.000	0.000	2.630	−7.053
0	−6	3	0.724	−6.000	3.000	2.677	−7.039
0	6	3	0.276	6.000	3.000	2.677	−7.055
0	0	−3	−0.500	0.000	−3.000	2.858	−7.049
−1	7	−2	−1.252	7.000	−2.000	2.872	−7.043
−1	1	4	−0.532	1.000	4.000	2.872	−7.051
0	10	1	0.045	10.000	1.000	2.915	−7.053
0	−2	4	0.563	−2.000	4.000	2.915	−7.044
1	3	−3	0.594	3.000	−3.000	2.986	−7.044
1	−3	−3	0.406	−3.000	−3.000	2.986	−7.054
0	−8	−2	−0.770	−8.000	−2.000	3.082	−7.058
0	4	4	0.378	4.000	4.000	3.082	−7.057
0	−10	2	0.872	−10.000	2.000	3.136	−7.050
0	−10	−1	−0.872	−10.000	−1.000	3.136	−7.058
−1	−11	1	−0.041	−11.000	1.000	3.202	−7.056
−1	−5	4	−0.351	−5.000	4.000	3.202	−7.047
1	−9	3	1.788	−9.000	3.000	3.304	−7.050
1	9	3	1.212	9.000	3.000	3.304	−7.060
0	6	−3	−0.327	6.000	−3.000	3.342	−7.049
0	−6	−3	−0.673	−6.000	−3.000	3.342	−7.062
1	11	−1	0.883	11.000	−1.000	3.403	−7.055
1	11	2	1.117	11.000	2.000	3.403	−7.062

TABLE II. Positions and energies of atoms around complete screw dislocation.

Identity			Coordinates x	y	z	Distance from the center in nearest-neighbor distances (Å)	Energy E_i (eV)
0	0	0	−0.307	0.000	0.000	0.408	−6.763
−1	1	1	−0.804	1.000	1.000	0.500	−6.689
0	−2	1	0.702	−2.000	1.000	0.707	−6.755
1	3	0	0.780	3.000	0.000	0.957	−7.038
1	−3	0	0.201	−3.000	0.000	0.957	−6.700
0	4	1	0.033	4.000	1.000	1.225	−6.992
1	−1	−1	0.604	−1.000	−1.000	1.258	−7.039
1	−1	2	1.616	−1.000	2.000	1.258	−7.031
0	2	−1	−0.312	2.000	−1.000	1.354	−7.049
0	2	2	0.358	2.000	2.000	1.354	−6.991
−1	−5	1	−0.201	−5.000	1.000	1.500	−7.037
0	−4	2	0.719	−4.000	2.000	1.683	−7.046
0	−4	−1	−0.640	−4.000	−1.000	1.683	−6.996
0	−6	0	−0.957	−6.000	0.000	1.780	−6.994
0	6	0	−0.196	6.000	0.000	1.780	−7.053
1	5	−1	0.720	5.000	−1.000	1.893	−7.059
1	5	2	1.196	5.000	2.000	1.893	−7.023
0	0	3	0.591	0.000	3.000	2.041	−7.050
−1	7	1	−1.038	7.000	1.000	2.062	−7.038
−1	1	−2	−1.360	1.000	−2.000	2.062	−7.060
0	−2	−2	−0.429	−2.000	−2.000	2.121	−7.055
1	−3	3	1.682	−3.000	3.000	2.217	−7.057
1	3	3	1.427	3.000	3.000	2.217	−7.038
0	−8	1	0.831	−8.000	1.000	2.345	−7.053
0	4	−2	−0.329	4.000	−2.000	2.345	−7.064
1	−7	2	1.777	−7.000	2.000	2.363	−7.059
1	−7	−1	0.203	−7.000	−1.000	2.363	−7.025
−1	−5	−2	−1.573	−5.000	−2.000	2.500	−7.045
0	8	2	0.103	8.000	2.000	2.614	−7.039
0	8	−1	−0.264	8.000	−1.000	2.614	−7.061
1	9	0	0.809	9.000	0.000	2.630	−7.056
1	−9	0	−0.018	−9.000	0.000	2.630	−7.045
0	−6	3	0.739	−6.000	3.000	2.677	−7.062
0	6	3	0.292	6.000	3.000	2.677	−7.040
0	0	−3	−0.396	0.000	−3.000	2.858	−7.062
−1	7	−2	−1.305	7.000	−2.000	2.872	−7.066
−1	1	4	−0.418	1.000	4.000	2.872	−9.055
0	10	1	−0.078	10.000	1.000	2.915	−7.048
0	−2	4	0.658	−2.000	4.000	2.915	−7.060
1	3	−3	0.637	3.000	−3.000	2.986	−7.066
1	−3	−3	0.552	−3.000	−3.000	2.986	−7.060
0	−8	−2	−0.701	−8.000	−2.000	3.082	−7.041
0	4	4	0.462	4.000	4.000	3.082	−7.050
0	−10	2	0.813	−10.000	2.000	3.136	−7.062
0	−10	−1	−0.888	−10.000	−1.000	3.136	−7.041
−1	−11	1	−0.137	−11.000	1.000	3.202	−7.060
−1	−5	4	−0.296	−5.000	4.000	3.202	−7.064
1	−9	3	1.774	−9.000	3.000	3.304	−7.065
1	9	3	1.201	9.000	3.000	3.304	−7.050
0	6	−3	−0.330	6.000	−3.000	3.342	−7.067
0	−6	−3	−0.542	−6.000	−3.000	3.342	−7.056
1	11	−1	0.759	11.000	−1.000	3.403	−7.062
1	11	2	1.045	11.000	2.000	3.403	−7.048

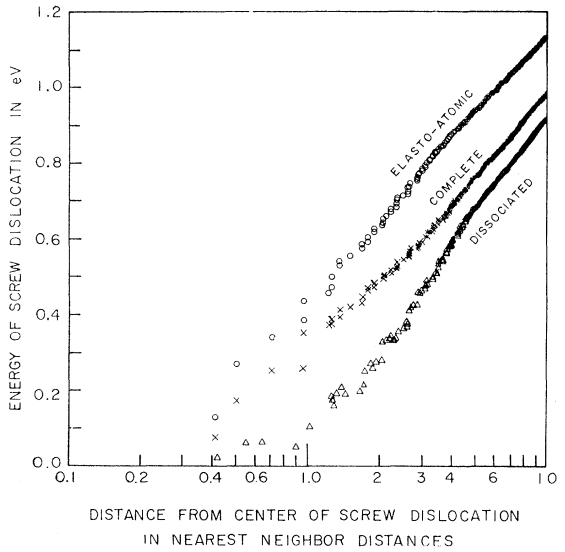

FIG. 4. Energy within a given radius as a function of that radius as measured from the center of a screw dislocation. The three cases, elasto-atomic, complete, and dissociated, are shown.

of the linear region of the curve [which would be in agreement with Eqs. (3) and (5)] can be seen.

B. Dissociated Screw Dislocation

After the calculations on the complete screw dislocation were completed, the final positions of the atoms were fed back into the computer and further relaxations were permitted, this time with the limitations against movements perpendicular to the dislocation line removed. The complete dislocation dissociated spontaneously. The positions of the atoms near the dissociated dislocation are shown in Fig. 3(c) [which should be compared with Figs. 3(a) and 3(b)]. The two partial dislocations can be distinguished in Fig. 3(c); and by comparing the positions of the atoms with respect to the fiduciary triangles in the last two sections of Fig. 3, and noting that the open circles suffer a displacement in the ⟨112⟩ direction. It can be seen that the region between them is a stacking fault. The separation distance between the partials is approximately 12 Å or $5b$. The reasons why (as in the case of the edge dislocation) this separation distance might not reflect the true situation in copper are discussed in Sec. V. The positions of the atoms surrounding the dissociated screw dislocation are given in Table III.

The energy of the dissociated dislocation is plotted as a function of radius in Fig. 4. The drop in energy during dissociation is the vertical distance between the asymptotic regions of the complete atomistic and dissociated atomistic curves. As was noted earlier, this energy change will be in error if, as is quite likely, the distance of separation of the partials is not correctly given by the calculation. This error is discussed in Sec. V. It is shown in that section that the separation distance is probably underestimated, and the dissociation energy

TABLE III. Positions and energies of atoms around dissociated screw dislocation.

Identity			Coordinates x	y	z	Distance from the center in nearest-neighbor distances (Å)	Energy E_i (eV)
0	0	0	−0.504	−0.219	−0.006	0.418	−6.970
−1	1	1	−0.606	1.228	1.022	0.555	−6.897
0	−2	1	0.576	−1.789	0.990	0.653	−7.059
1	3	0	0.637	2.813	0.017	0.903	−7.119
1	−3	0	0.293	−3.218	−0.033	1.026	−6.847
0	4	1	0.202	4.202	1.033	1.289	−6.836
1	−1	−1	0.490	−1.079	−1.011	1.272	−7.016
1	−1	2	1.554	−0.925	1.999	1.252	−7.028
0	2	−1	−0.395	1.929	−0.992	1.339	−7.038
0	2	2	0.314	2.092	2.022	1.382	−6.998
−1	−5	1	−0.306	−4.841	0.982	1.452	−7.142
0	−4	2	0.655	−3.928	1.986	1.661	−7.039
0	−4	−1	−0.659	−4.094	−1.029	1.719	−6.992
0	−6	0	−0.874	−6.172	−0.028	1.833	−6.854
0	6	0	−0.263	5.874	0.013	1.741	−7.142
1	5	−1	0.693	4.931	−0.987	1.871	−7.043
1	5	2	1.273	5.096	2.029	1.929	−6.997
0	0	3	0.539	0.025	3.002	2.043	−7.058
−1	7	1	−0.931	7.144	1.020	2.106	−6.889
−1	1	−2	−1.420	0.981	−1.998	2.059	−7.059
0	−2	−2	−0.514	−2.030	−2.010	2.132	−7.052
1	−3	3	1.624	−2.979	2.993	2.210	−7.057
1	3	3	1.430	3.041	3.017	2.235	−7.040
0	−8	1	0.782	−7.905	0.991	2.317	−7.131
0	4	−2	−0.346	3.980	−1.993	2.337	−7.053
1	−7	2	1.734	−6.936	1.989	2.342	−7.046
1	−7	−1	0.215	−7.085	−1.025	2.395	−7.009
−1	−5	−2	−1.627	−5.046	−2.021	2.522	−7.033
0	8	2	0.168	8.077	2.019	2.641	−7.023
0	8	−1	−0.239	7.942	−0.992	2.596	−7.050
1	9	0	0.810	8.931	0.004	2.610	−7.116
1	−9	0	0.027	−9.113	−0.013	2.664	−6.929
0	−6	3	0.692	−5.976	2.992	2.667	−7.052
0	6	3	0.321	6.049	3.021	2.699	−7.034
0	0	−3	−0.447	−0.001	−3.001	2.858	−7.061
−1	7	−2	−1.285	6.977	−1.994	2.864	−7.052
−1	1	4	−0.479	1.005	4.004	2.875	−7.062
0	10	1	0.000	10.090	1.007	2.942	−6.963
0	−2	4	0.593	−1.999	3.997	2.913	−7.061
1	3	−3	0.617	2.999	−2.996	2.983	−7.062
1	−3	−3	0.477	−3.010	−3.009	2.994	−7.059
0	−8	−2	−0.727	−8.046	−2.019	3.102	−7.040
0	4	4	0.436	4.017	4.012	3.093	−7.053
0	−10	2	0.795	−9.951	1.995	3.121	−7.054
0	−10	−1	−0.872	−10.063	−1.014	3.157	−7.035
−1	−11	1	−0.156	−10.953	0.999	3.188	−7.100
−1	−5	4	−0.347	−4.997	3.995	3.198	−7.060
1	−9	3	1.748	−8.976	2.995	3.296	−7.050
1	9	3	1.233	9.042	3.014	3.321	−7.047
0	6	−3	−0.327	5.996	−2.996	3.338	−7.057
0	−6	−3	−0.611	−6.021	−3.015	3.355	−7.048
1	11	−1	0.814	10.959	−0.998	3.392	−7.057
1	11	2	1.098	11.054	2.009	3.421	−7.043

derived from Fig. 4 (i.e., about 0.08 eV per {110} plane) is a lower limit.

V. DISCUSSION

It can be seen from Fig. 3(b) that the complete screw dislocation is not very wide. Formally, the width is defined as being the range of x within which the displacement is less than one-half of its limiting value (i.e., $-b/8 \leqslant u(x) \leqslant b/8$).[10,11] Using this criterion, the dislocation in the present study is found to have a width of about 2 b.

The energy plot of Fig. 4 is, of course, directly related to Fig. 1. The point at which the atomistic curve deviates from a straight line is equivalent to the point at which the solid and dashed lines meet in Fig. 1 (i.e., the point at which $r=r_C{}^s$). Thus the core radius can be read off directly from Fig. 4 and one gets a value

$$r_C{}^s = 2.1 d_0. \tag{12}$$

Furthermore, the energy at that point is equivalent to the horizontally shaded region of Fig. 1 and is simply the core energy. In the present case this is

$$E_{\text{core}}{}^s = 0.5 \text{ eV per } d_0/2. \tag{13}$$

Finally, it will be noted that the intercept on the $\ln r$ axis of the extrapolated straight-line region in Fig. 4 is equal to $r_{\text{eh}}{}^s$, the equivalent hole radius in Fig. 1. This is found to be

$$r_{\text{eh}}{}^s = 0.44 d_0. \tag{14}$$

A calculation of the dislocation energy using the elastic-continuum equation (9) and this value of $r_{\text{eh}}{}^s$ would automatically take into account the true energy of the core.

As in Paper I, the term *cutoff radius* has not been used. This is to avoid ambiguity because that term can validly be applied to both $r_C{}^s$ and $r_{\text{eh}}{}^s$. On the other hand, the terms *core radius* and *equivalent hole radius* are quite unambiguous and can be applied to these two radii, respectively, without any risk of confusion.

The spontaneous dissociation of the screw dislocation, when the atoms are allowed to move in a direction perpendicular to the dislocation line, is demonstrated by the difference between Figs. 3(b) and 3(c). The equilibrium separation distance of the partial dislocations is achieved when the replusive force between them is just balanced by the attractive force of the stacking fault which separates them. If conditions were such that no other factors affected the separation, one could, in principle, make an estimate of the stacking-fault energy using this distance.

The magnitude of the force per unit length between two parallel, infinite, complete, pure edge dislocations is[12]

$$F^E = \mu b_1{}^E b_2{}^E / 2\pi(1-\nu) r, \tag{15}$$

where b_1 and b_2 are the Burgers vectors of the respective dislocations, and r is the distance of separation. The corresponding force between screw dislocations is

$$F^s = \mu b_1{}^s b_2{}^s / 2\pi r. \tag{16}$$

For a dissociated screw dislocation the partials have both edge and screw components, where $b_1{}^E = d_0/2\sqrt{3}$, $b_2{}^E = -d_0/2\sqrt{3}$, $b_1{}^s = d_0/2$, and $b_2{}^s = d_0/2$. The force per unit length between the partials, when they are separated by a distance r, is

$$F = F^E + F^s = \frac{-\mu d_0{}^2}{24\pi(1-\nu) r} + \frac{\mu d_0{}^2}{8\pi r}. \tag{17}$$

The force per unit length due to the stacking fault is simply $-\gamma$. Thus the total force trying to separate the partials is

$$F^{\text{total}} = \frac{\mu d_0{}^2}{8\pi r}\left\{\frac{-1}{3(1-\nu)} + 1\right\} - \gamma. \tag{18}$$

Equating F_{total} to zero, we obtain the equilibrium separation of the partials, $r_{\text{eh}}{}^s$

$$r_{\text{eq}}{}^s = \frac{\mu d_0{}^2}{24\pi\gamma}\left\{\frac{2-3\nu}{1-\nu}\right\}. \tag{19}$$

Using the experimental values for copper, $\mu = 4.9 \times 10^{11}$ dyn cm^{-2}, $d_0 = 2.5$ Å, $\gamma \simeq 60$ erg cm^{-2}, and $\nu = 0.3$, we obtain

$$r_{\text{eq}}{}^s \simeq 8 \text{ Å}. \tag{20}$$

In the present calculations, however, there are at least two reasons why the separation distance might be in error. It must be noted that the present calculations are strictly applicable only to the absolute zero temperature so that the two partials have no chance of overcoming the Peierls-Nabarro barrier.[13,14] The situation is shown in Fig. 5, and there are three energy components to be considered. The stacking-fault term increases linearly with separation, while the interaction term falls asymptotically to zero. The Peierls-Nabarro energy is periodic (but, of course, is not necessarily sinusoidal). Summing up these three contributions, we obtain the net-energy curve shown at the bottom of the figure. It can be seen from the figure that even at the absolute-zero temperature the complete dislocation will move to position A. This position is probably the one which is achieved by the second partial dislocation in the present calculations. At a finite temperature the partial could move to position B, and eventually by a series of jumps to C, by a thermally activated process. The second source of error concerns the stacking-fault term itself. If the stacking fault which appears between the partials is to play its proper role in determining the separation distance, the stacking-fault energy predicted by the model would have to match the true value of that parameter. This poses considerable difficulty. Details of a calculation of the stacking-fault energy of copper based on the Morse potential are given in Paper I. It has been shown that the calculated stacking-fault energy

[10] Reference 4, p. 61.
[11] A. J. Foreman, M. A. Jaswon, and J. K. Wood, Proc. Phys. Soc. (London) **A64**, 156 (1951).
[12] Reference 4, p. 45.
[13] R. Peierls, Proc. Phys. Soc. (London) **52**, 34 (1940).
[14] F. R. N. Nabarro, Proc. Phys. Soc. (London) **59**, 256 (1947).

depends upon the truncation of the potential.[1] For no truncation the value is close to 1 erg cm^{-2}. This is only about 2% of the experimental value for copper. Truncation at 176 neighbors gives an "artificial" value of 30 erg cm^{-2}. This is why this truncation was used in the present calculations.

It is interesting to note that, by use of Eqs. (6) and the corresponding equation for the edge dislocation,

$$E^E(r)=\frac{\mu b^2}{4\pi(1-\nu)}\ln\frac{r}{r_{\mathrm{eh}}{}^E}, \tag{21}$$

together with the observed asymptotic slopes of the curves shown in Fig. 4 and the corresponding curve for the edge dislocation, atomistic values of μ and ν may be derived. The asymptotic slope of the complete atomistic edge dislocation is 0.59 eV per {112} plane (i.e., per distance $d_0/2\sqrt{3}$),[1] and from Fig. 4 the corresponding slope for the screw dislocation is 0.73 eV per {110} plane (i.e., per distance $d_0/2$). From Eq. (6) the slope for the screw dislocation is $\mu b^2/4\pi$, and μ is the only unknown quality. Thus we have

$$\mu=18.8\times10^{11}\text{ dyn cm}^{-2}. \tag{22}$$

From Eq. (21) the slope for the edge dislocation is $\mu b^2/4\pi(1-\nu)$. Thus the ratio of the slopes is $(1-\nu)$, from which one obtains

$$\nu=0.28. \tag{23}$$

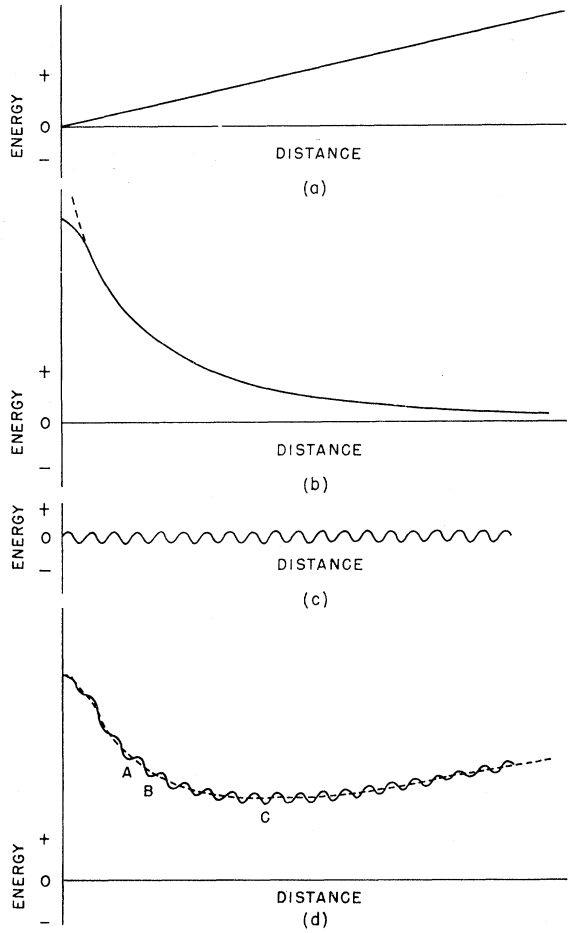

FIG. 5. Schematic plot of the relative energies of a system of two partial dislocations separated by a stacking fault. The relative energies are shown as a function of the distance separating the partials. The first three curves show the separate components arising from (a) the stacking fault, (b) the interaction between the partials, and (c) the Peierls-Nabarro barrier. Curve (d) is the result of summing the various components.

VI. SUMMARY

The investigation described in this paper shows that a realistic three-dimensional crystal model of an atomistic screw dislocation can be constructed within the framework of the central-force approximation. The calculations were specifically for copper, but they could easily be extended to other fcc metals. Moreover, with minor modifications this method could be extended to other crystal structures. This might well shed some light on the as yet not-well-understood properties of dislocations in such crystals.

The dislocation studied here was the screw dislocation in copper. A variational method was employed, and the pairwise interaction between discrete atoms was represented by a Morse potential function. The calculations were carried out on a digital computer. For the complete screw dislocation it was necessary to artificially prevent atoms from moving in a direction normal to the dislocation line. This prevented dissociation. For a complete dislocation (Burgers vector $(a_0/2)\langle110\rangle$) linear elastic theory breaks down inside a *core radius* of 5.3 Å. The core energy, 1.0 eV per nearest-neighbor distance, is in good agreement with previous rough estimates. If the core is replaced by a cylindrical hole of radius r_{eh} (the *equivalent hole radius*), the inside of which is hollow and outside of which linear elastic theory holds at all points, this radius is 1.1 Å. The complete dislocation has a width of 5 Å (i.e., $2b$).

When the atoms are allowed to relax in the directions normal to the dislocation line, spontaneous dissociation into two Heiderneich-Shockley partials occurs, with no activation energy.

A comparison between the asymptotic behavior of energies of the edge and screw dislocations at large radii permitted atomistic values of the shear modulus and Poisson's ratio to be calculated. These values were 18.8×10^{11} dyn cm^{-2} and 0.28, respectively, for copper.

A brief account of these calculations has been published earlier.[15,16]

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[15] M. Doyama and R. M. J. Cotterill, Phys. Letters **13**, 110 (1964).

[16] R. M. J. Cotterill and M. Doyama, Phys. Letters **14**, 79 (1965).