#74

PHYSICAL REVIEW B VOLUME 26, NUMBER 10 15 NOVEMBER 1982

Energy and entropy of interacting dislocations

Anthony J. C. Ladd
Department of Applied Science, University of California at Davis, Davis, California 95616

William G. Hoover
Lawrence Livermore National Laboratory, Livermore, California, 94550
and Department of Applied Science, University of California at Davis-Livermore,
Livermore, California 94550

(Received 29 January 1982; revised manuscript received 19 April 1982)

The energy and entropy of interacting edge dislocations have been calculated by atomistic simulations, with the use of piecewise-linear forces in a two-dimensional triangular lattice. We conclude that the interaction energy between small groups of dislocations is well described by continuum mechanics for separations greater than a few lattice spacings. Our calculations enable us to make a precise determination of the core energy, which is an essential parameter in determining dislocation multiplication rates. We find also that continuum mechanics gives an accurate representation of the interaction of a dislocation pair with a homogeneous elastic stress field. The vibrational contribution to the entropy of such a pair is small, about $0.3k$.

I. INTRODUCTION

Plastic flow occurs, primarily, through the motion of edge dislocations. The importance of dislocations in plastic flow stems from their mobility, and low energy of formation, which makes it possible to create large numbers of them during plastic deformation. However, there has been little theoretical attention paid to these two properties, despite the scientific and technological interest in a quantitative understanding of the relationship between dislocations and plastic flow.

Phenomenological models calculate the "plastic strain rate" in terms of the density, velocity, and mobile fraction of dislocations.[1] The parameters in these models are not directly related to the properties of individual dislocations, but are determined by fitting the predictions of the model to experimental data. This approach has been successful in correlating experimental data, but only by using different constitutive laws for different strain-rate regimes. Consequently, the predictive power of these models is limited. In addition, these theories have been unable to explain, consistently, the large plastic relaxation observed behind weak shock waves in LiF single crystals.[2]

The elastic theory of dislocations[3] is insufficient for a complete description of plastic flow. It predicts stress-field divergences in the dislocation-core region, where a precise knowledge of the finite forces is necessary for a quantitative description of dislocation creation and annihilation. Although the release of elastic strain energy is the driving force for dislocation motion, an effective mass of a dislocation cannot be calculated from first principles. The equations of motion of dislocations must, therefore, be determined from computer simulation or etch-pit experiments.[1] These results indicate that dislocations accelerate extremely rapidly to a constant velocity characteristic of the local stress. The time spent in nonuniform motion is short, typically a few Einstein vibrational periods. For dislocations traveling at one-half the transverse sound speed, this corresponds to a distance of about one lattice spacing.

Calculation of the atomic displacements in the dislocation core is difficult, even in the linear approximation. Early efforts are exemplified by the peculiar Frenkel-Kontorova model and the more realistic Peierls-Nabarro model.[3,4] Recent efforts have concentrated on the analytically more tractable screw dislocation.[5] Edge dislocations are mathematically more complicated, but they dominate plastic flow in three dimensions as well as being the only type of dislocation that can exist in two dimensions.

The advent of fast computers has made it possible to study the properties of a small number of dislocations exactly. Computer simulations have been used to study the core structure of edge dislocations in the triangular[6] and face-centered-cubic lattices,[4,7] dislocation glide and climb,[6] and the interaction between pairs of dislocations.[8] Computer simulations are limited to regions less than 100 atomic spacings wide and to times less than 10^5 vibrational periods. The resolution of experimental shock-wave physics is limited to lengths and times that are somewhat larger than atomic spacings and vibration periods.[9] These two classes of experiment are thus complementary, so that achieving correlations between them can lead to an increased understanding of plastic flow in real materials. Comparisons between microscopic molecular dynamics and macroscopic Navier-Stokes simulations of strong shockwaves in dense monatomic fluids have already been made.[10] The equation of state and the transport coefficients used in the Navier-Stokes solution were obtained by molecular dynamics simulations as well. The results of the two calculations were in encouragingly good agreement, even for strong shocks that result in final densities of twice the initial triple-point density. The absence of a solid-flow equivalent to the Navier-Stokes equation is a serious hindrance to studies of plasticity.

As a first step towards understanding plastic flow at high strain rates, we have carried out molecular dynamics simulations of simple crystals undergoing steady isothermal shear.[11] From these calculations we obtain constitutive equations for the stress and energy as a function of plastic strain rate and temperature. Most of these simulations involved the two-dimensional triangular lattice described below, but some calculations sheared a three-dimensional close-packed lattice. In both cases piecewise-linear forces were used. It seems implausible that plastic flow can depend in a fundamental way on such details as the crystal structure or interatomic force law. We have found that the shear stress in both two- and three-dimensional crystals is well represented by a power-law dependence on strain rate of the form $\sigma \propto \dot{\epsilon}^p$, where $\dot{\epsilon}$ is the strain rate. The parameter p is temperature dependent. At low temperatures $p \sim 0.1$ where the flow is close to being perfectly plastic and near melting $p \sim \frac{1}{2}$. Such power-law dependences of the stress on strain rate are often observed experimentally.[12] There is semiquantitative agreement between the results of the computer simulations in both two- and three-dimensions and experimental results deduced from strong shock waves in aluminum.[13] Although there has been considerable theoretical effort devoted to theories of plastic flow based on dislocation motion,[14] there have been few quantiative results that can be compared with experiment. A notable exception is the work of Werne,[15] which incorporates a dislocation-based model of plastic flow into continuum solid-mechanics simulations of simple mechanical tension tests. We are investigating the applicability of dislocation theory to computer simulations of plastic flow at high strain rates. A necessary preliminary is the ability to describe the energy and stress of crystals containing dislocations. This is the subject of the present paper.

Plastic flow in the triangular lattice incorporates the creation, interaction, motion, and annihilation of crystal defects without the geometrical complexities involved in three-dimensional crystals. The possible dislocation reactions in the triangular lattice are illustrated in Fig. 1. This geometrical simplicity together with the elastic isotropy and mechanical stability with just near-neighbor forces makes this lattice ideal for initial studies of plastic flow.

It has been found that linear forces result in small, stable dislocation cores with large Peierls strains.[6] This means that stable dislocation pairs can be created at small separations (four or five lattice spacings), and the results of atomic and continuum mechanics compared. In view of the size limitations of atomic calculations this is a very desirable feature. By comparison, use of the Lennard-Jones potential results in extended cores and much small-

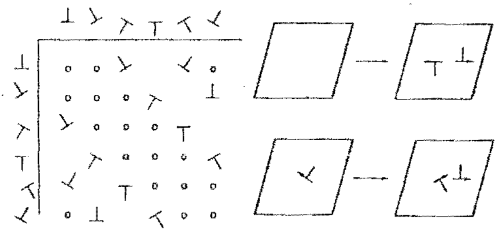

FIG. 1. Dislocation reactions in a triangular lattice. There are three glide directions in a triangular lattice orientated at angles of 120°, 240°, and 360°, and thus six orientations for edge dislocations. The dislocation reaction matrix is shown on the left-hand side of the figure. The reaction can proceed in either direction. A zero indicates that it is not a geometrically possible reaction and a blank space indicates a perfect lattice. The right-hand side shows dislocation production in a sheared crystal. The direction of the shear is the one that is most favorable for the reactions shown. The arrows on the dislocations indicate the direction of glide of the dislocations if the external shear is larger than the attractive force between the pair.

Peierls strains. In addition the number dependence of the propagation velocity is reduced with soft linear forces.[6] We use a piecewise-linear force law,

$$\phi(r)=\begin{cases}\frac{1}{2}\kappa(r-d_0)^2-\kappa w^2\ , & r\le d_0+w\\ -\frac{1}{2}\kappa(r-d_0-2w)^2\ , & d_0+w<r\le d_0+2w\\ 0, & d_0+2w<r\end{cases} \quad (1)$$

where d_0 is the interatomic distance in the strain-free lattice, and κ is the force constant. We use a value of $w=0.15d_0$, corresponding to one broken bond in the dislocation core of a lattice with stress-free boundaries.[6] The thermodynamic properties of this lattice over a range of densities have been calculated.[16]

According to linear elastic theory, the energy of a two-dimensional array of n edge dislocations in an isotropic continuum at constant pressure is

$$E=nE_c+D\sum_{i>j}\left[-(\vec{b}_i\cdot\vec{b}_j)\ln(r_{ij}/b)+(\vec{b}_i\cdot\vec{r}_{ij})(\vec{b}_j\cdot\vec{r}_{ij})/r_{ij}^2\right]\ , \quad (2)$$

where E_c is the core energy of a dislocation and D is given in terms of the Lamé constants by

$$D=(\eta/\pi)(\lambda+\eta)/(\lambda+2\eta)\ .$$

For the triangular lattice with Hooke's-law forces, the Lamé constants are given by[16]

$$\eta=(\sqrt{3}/4)(4-3\rho^{1/2})\ ,$$
$$\lambda=(\sqrt{3}/4)(5\rho^{1/2}-4)\ , \quad (3)$$

where ρ is the density relative to the stress-free density.

The total Burgers vector $\vec{B}=\sum_{i=1}^{n}\vec{b}_i$ is conserved during plastic deformation. Consequently, the term $B\ln V$ is unchanged during a shear deformation and is, therefore, not included in Eq. (2). Furthermore, the core radius r_c and core energy E_c are not independent. We choose $r_c=b$. The primary purpose of this work is to test the validity of the elastic theory at separations of a few atomic diameters, and to determine, if possible, a consistent value for the core energy in the Hooke's-law triangular lattice.

Our calculations use groups of two or three dislocations in a triangular lattice arranged so that $B=0$ (Fig. 2). The strain energy is small, and tends to a finite limit as the crystal gets large. This permits an accurate determination of the core energy, which is typically an order of magnitude larger than the interaction energy. The displacement fields obtained from elastic theory are not unambiguous, but depend on the short-range and long-range boundary conditions.[4] We therefore use periodic boundary conditions, with a hexagonal unit cell, which is superior to a rectangular one, because the latter introduces an N-dependent elastic anisotropy. Typical arrangements of dislocations are shown in Fig. 2.

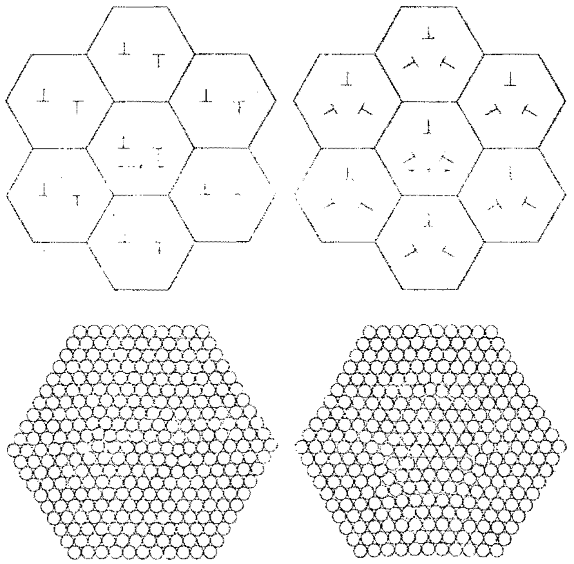

FIG. 2. Periodic arrays of dislocations. The upper half of the figure shows seven cells of the infinite periodic array. The dislocation separation is indicated. The lower half of the figure shows typical arrangements in fully relaxed unit cells.

Most atomic simulations have focused on details of the core structure in various crystals containing a single dislocation.[4,7] The energy of such crystals diverges logarithmically with system size and contains a constant term that depends on the exact nature of the imposed boundary conditions. It is not possible, therefore, to determine a core energy from such a calculation that can then be used to characterize the energy of a plastically flowing crystal. More recently, a core energy has been estimated from simulations of pairs of dislocations in the two-dimensional electron solid.[8] The core energies obtained from the various pair arrangements were not very consistent, varying by factors up to 1.6.

Our calculations involve several different system sizes, ranging from about 10^2 to 10^3 atoms, for the same dislocation arrangements. The arguments given in Ref. 8 predict that the energy N dependence will vary as N^{-1}, where N is the number of atoms. This means we can extrapolate our results to the large-system limit and estimate the errors in doing so. In addition, we have used elastic theory to estimate directly the effects of the periodic boundaries on the energy of small crystals.

II. RESULTS

A. Relaxation

The initial conditions were obtained by using the results of elastic theory for the displacement fields around a dislocation.[3] The location of each dislocation was chosen to minimize the displacements in the core region. The two arrangements used are shown in Fig. 2. For the triangular arrangement, the periodic boundary conditions require the removal of a small number of atoms. We then adjusted the volume to maintain a constant density, as this resulted in smaller number dependencies.

The relaxation was carried out using the equations of motion of a damped harmonic oscillator.

$$\ddot{x}+2\lambda\dot{x}+\omega_0^2x=0\ . \tag{4}$$

For a single oscillator of frequency $\omega_0=(\kappa/m)^{1/2}$, the optimal value of the damping factor λ is ω_0, which results in exponential damping. For a collection of oscillators, λ is chosen to damp the low-frequency modes. We have found, empirically, that $\lambda=\omega_0/L$, where L is the number of atoms on the side of the hexagon, is a suitable choice.

We used Verlet's scheme, which for damped equations of motion is

$$\begin{aligned}(x_+-x_0)&=[(x_0-x_-)(1-\lambda\Delta t)\\&\qquad+(F_0/m)\Delta t^2]/(1+\lambda\Delta t)\ ,\\ v_0&=(x_+-x_-)(2\Delta t)\ ,\end{aligned}\tag{5}$$

with a time step $\Delta t=0.1\omega_0^{-1}$. Typically 10^3 time steps were required to reduce the magnitudes of the forces to less than $10^{-8}\kappa d_0$.

B. Energies of dislocation pairs and triplets

Preliminary calculations were carried out at the strain-free density, $\rho=(\sqrt{3}/2)Nd_0^2/V=1$, with a pair of dislocations, of opposite sign, on the same glide plane, at a separation of $6d_0$ [Fig. 2(a)]. Crystals with 6, 7, 8, and 10 atoms on a side were used, corresponding to unit cells of 108, 147, 192, and 300 atoms. Both periodic and stress-free boundary conditions were used as a numerical check of the extrapolation procedure. Linear extrapolation gave infinite-system energies for the pair $E(6d_0)$ of $0.256\kappa d_0^2$ and $0.252\kappa d_0^2$ for the stress-free and periodic boundaries, respectively. In order to obtain more accurate extrapolated results at the density ρ of 1.1, crystals of up to 972 atoms per unit cell were used, together with higher-order polynomial fits. The errors were estimated from the consistency of the extrapolated energy derived from the various fits.

The energies of various arrangements of dislocations in different sized systems are shown in Table I. From the initial conditions that we used, it was impossible to obtain relaxed configurations with dislocations pairs closer than $6d$, where $d/d_0=\rho^{-1/2}$, nor was it possible in the two smallest systems to obtain relaxed configurations with dislocations pairs at $12d$. A plot of energy vs $1/N$ is shown in Fig. 3 for pairs of dislocations at separations between $6d$ and $12d$. It can be seen that the energy is essentially linear in $1/N$ with small corrections from higher-order terms. The N dependence is large and varies strongly with the dislocation separation and arrangement. For the triangular arrangements, the N dependence has the opposite sign to that for the pair arrangements. Thus, unless the N-dependent contribution can be calculated accurately, it is essential to extrapolate the dislocation energies to the infinite-system limit before making comparisons with elasticity theory.

For all the pair configurations, the data is almost exactly fitted by a quadratic polynomial in $1/N$. The extrapolated energies are consistent to within the error bars with those obtained from higher-order polynomial fits. In Fig. 3 we show the linear $(1/N)$ deviations from the infinite-system results, based on the polynomial fits. The quadratic deviations are significant for crystals less than about 500 atoms. The results at $12b$ are much less precise, and the error bars in this case may be underestimated. The N dependence is largest for this system and we only have results for three crystal sizes. For the triangular arrangement, the agreement between the quadratic and higher-order fits is not as good especially when $r=8b$. The error bars are consequently larger. Our estimates of the extrapolated energies, together with probable error bars, are shown in Table II.

Some crystals were relaxed in the presence of a homogeneous external shear strain ϵ by applying a volume-conserving displacement $x\rightarrow x+\epsilon y$ to each atom in the lattice. We use pairs of dislocations at separations of $2d$ and $4d$, and crystals of 75, 108,

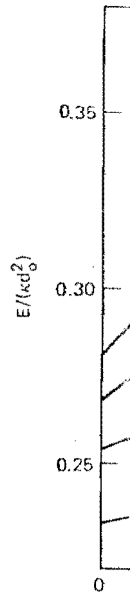

FIG. Ene
crystals p
our estimates o
gies of a disloca

TABLE I. Energies of dislocations in finite-size crystals. The subscripts 2 and 3 refer to the pair and triangular arrangements. The dislocation energies are given relative to the energy of a perfect lattice at the same density, $\rho=1.1$.

r/b	N_2	$E_2/\kappa d_0^2$	N_3	$E_3/\kappa d_0^2$
4			184	0.428 354
			292	0.449 681
			424	0.460 448
			964	0.473 073
6	192	0.263 837	180	0.398 712
	243	0.256 528		
	300	0.251 534	288	0.449 432
	432	0.245 366	420	0.475 175
	972	0.238 204	960	0.504 713
8	192	0.314 571	176	0.333 342
	243	0.300 136		
	300	0.290 196	284	0.417 497
	432	0.277 979	416	0.464 665
	972	0.264 164	956	0.519 717
10	192	0.370 070		
	243	0.347 639		
	300	0.331 203		
	432	0.310 391		
	972	0.286 824		
12	300	0.375 462		
	432	0.344 854		
	972	0.308 297		

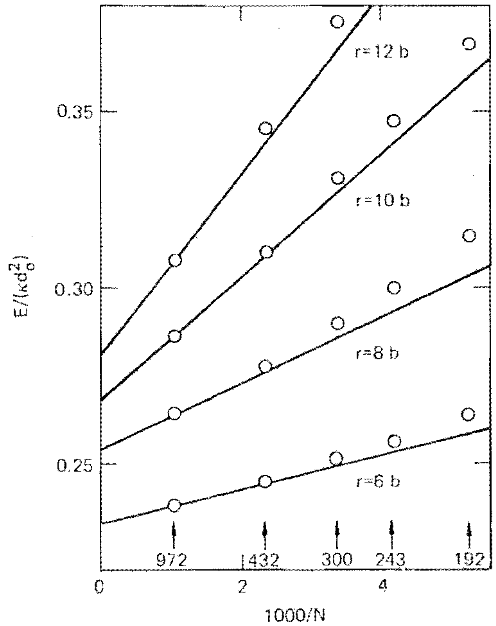

FIG. 3. Energies of dislocation pairs in finite-size stals with $\rho=1.1$. The straight lines correspond to our estimates of the linear $(1/N)$ deviations of the energies of a dislocation pair from the infinite-system result.

and 192 atoms. We found that the energy of a pair of dislocations is a linear function of the applied strain, within $0.001\kappa d_0^2$, with a coefficient that is only weakly dependent on the number of atoms in the crystal. These coefficients, together with the range of shear strains for which the pair is stable, are summarized in Table III. The almost complete

TABLE II. Energy of interacting dislocations. These energies are obtained by extrapolating the dislocation energies of finite-size crystals. The error bars are estimated from the consistency of different polynomial fits. The asterisks indicate that these energies were obtained by first extrapolating results in homogeneously strained crystals to zero strain (see Table III).

r/b	$E_2/\kappa d_0^2$	$E_3/\kappa d_0^2$
2	$0.147\ \pm 0.001$*	
4	$0.200\ \pm 0.001$*	0.4825 ± 0.0005
6	0.2330 ± 0.0001	$0.526\ \pm 0.001$
8	0.2545 ± 0.0005	$0.560\ \pm 0.004$
10	$0.270\ \pm 0.002$	
12	$0.281\ \pm 0.002$	

TABLE III. Energy of dislocation pairs in a homogeneous strain field. The energies shown here are obtained by extrapolating the results for crystals that are homogeneously sheared, $x'=x+\epsilon y$, with a shear strain ϵ, which varies over the range $\epsilon_{\min}$ to $\epsilon_{\max}$. All the results can be fitted within $0.001\kappa d_0^2$ by an expression of the form $E_2(\epsilon)=E_2+\Delta E_2\epsilon$. Elastic theory predicts that $\Delta E_2=-\eta br$, which corresponds to coefficients of $-0.672\kappa d_0^2$ and $-1.34\kappa d_0^2$ for $r=2b$ and $4b$, respectively. At this density $\rho=1.1$, the Lamé constants are $\eta=0.370\kappa$ and $\lambda=0.539\kappa$. D [Eq. (2)] is 0.0836κ. The interparticle spacing $d=b=0.953d_0$.

r/b	N_2	$E_2/\kappa d_0^2$	$\Delta E_2/\kappa_0^2$	$\epsilon_{\min}$	$\epsilon_{\max}$
2	75	0.1546	−0.645	0.10	0.22
	108	0.1520	−0.645	0.08	0.20
	192	0.1496	−0.645	0.08	0.20
	∞	0.147	−0.645	0.08	0.20
4	75	0.2389	−1.34	0.02	0.22
	108	0.2263	−1.335	0.02	0.20
	192	0.214 578	−1.327	0.00	0.18
	∞	0.200	−1.32	0.00	0.16

absence of N dependence in these results indicates that the shear modulus of the cold crystal is essentially unaffected by dislocation densities of 1% or less. We can extrapolate the dislocation-pair energies to zero strain even for arrangements that are unstable at zero strain. Since the N dependence of the interaction energy is relatively small at these separations, we can obtain reasonable estimates of the energies of these arrangements in the infinite-system limit. These results have been added to Table II.

A graph of the variation of energy per dislocation with $\ln(r/b)$ is shown in Fig. 4. The straight lines correspond to the best fits that can be obtained with the slope $-D\vec{b}_1\cdot\vec{b}_2$ derived from elastic theory. In fitting these lines a larger weight was given to the points that were determined more accurately. For both the pair and the triangular arrangements, the data is consistent with these straight lines to within the errors involved in extrapolating to the large-system limit, which is always less than 1%. The two lines are parallel and represent an energy difference, $(1/3)E_3-(1/2)E_2$, of $0.060\kappa d_0^2$. Elastic theory predicts a constant difference of $0.057\kappa d_0^2$ [Eq. (2)]. The core energies resulting from the two calculations are in good agreement, also; $0.086\kappa d_0^2$ and $0.089\kappa d_0^2$ for the pair and triangular arrangements, respectively. Given this value for the core energy, elastic theory can be used to calculate the energy of an array of n interacting dislocations in an infinite system, with an accuracy of order $10^{-3}n\kappa d_0^2$. Reference 8 describes the difficulties involved in extending this calculation to dislocations in finite periodic crystals. Our direct calculations have resulted in core energies for nine different arrangements that are consistent within 2% of $0.087\kappa d_0^2$.

A dislocation moving in a stress field releases stored elastic energy, which is converted into heat. The homogeneous nucleation of a pair of dislocations is assisted by an applied shear stress, which reduces the energy of the pair by an amount $-b\sigma r$,

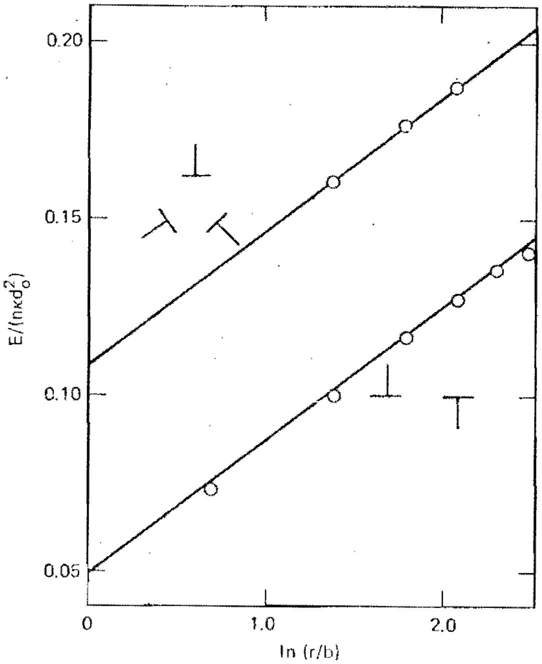

FIG. 4. Energies of dislocation groups with $\rho=1.1$. This figure shows the extrapolated energies per dislocation as a function of separation. The straight lines correspond to best fits consistent with the slope (0.0380) predicted by elastic theory. The intercepts are consistent to within $0.002\kappa d_0^2$ with a core energy per dislocation of $0.087\kappa d_0^2$.

where r is the separation of the pair. The stress σ is the external shear stress, resolved along the glide plane of the dislocation pair. In our atomic calculations, the "external shear stress" results from the displacement $x \rightarrow x + \epsilon y$, so that $\sigma = \eta\epsilon$. The coefficient, ΔE_2, of the stain-dependent energy, defined in Table III, is $-2\eta b^2$ and $-4\eta b^2$, according to elastic theory, for dislocations at separations of $2b$ and $4b$, respectively.

The actual coefficients determined from the atomic calculations are $-1.92\eta b^2$ and $-3.93\eta b^2$. Thus, the continuum theory results in a quantitative calculation of the energy of groups of dislocations in the presence of external stresses. The only parameter in this calculation is the core energy which has been determined for Hooke's-law forces as $0.087\kappa d_0^2 = 0.26\eta b^2$.

This paper has described a computational scheme, with which the energies of small groups of dislocations can be accurately determined. Our results are in good agreement with elastic theory and resulted in a core energy that is accurate to about $0.002\kappa d_0^2$. It should be emphasized that this accuracy is a minimum requirement for the quantitative prediction of dislocation multiplication rates in crystals undergoing plastic flow, which typically occurs at temperatures in the range $0.005-0.01\kappa d_0^2/k_B$. In the last two sections, we examine the applicability of elastic theory to calculations of the energy and stresses of dislocations in finite-size crystals.

C. Entropies of dislocation pairs

We have determined the entropies of 75- and 192-atom crystals containing a pair of dislocations at various separations, and with various external shear strains. The entropy is evaluated from the determinant of the force-constant matrix.[17] Two rows and two columns were deleted to remove the zero-frequency translational modes and the determinant was evaluated by Crout factorization.[18] The entropy of a pair of dislocations is then given by

$$\Delta S_{\rm vib}/k = \tfrac{1}{2}\ln(\det|\overleftrightarrow{F}'_0|/\det|\overleftrightarrow{F}'|)\ , \qquad (6)$$

where $\overleftrightarrow{F}'_0$ and $\overleftrightarrow{F}'$ are the perfect-crystal and dislocated-crystal force constant matrices, with two rows and two columns deleted. A useful check on the results is that they are independent of which rows and columns are deleted.

The vibrational entropy of a pair of dislocations (Table IV) is almost independent of the number of atoms in the crystals. This suggests that the frequency shifts are confined to modes that are localized around the dislocations. The entropy is weakly dependent on a homogeneous shear strain, varying by less than 2% for a 1% strain. It increases slowly with increasing separation of the dislocation pair and appears to be approaching a constant value of about $0.3k$ at large separations. The vibrational entropy of a dislocation pair is usually negative, but with Hooke's-law forces the elastic moduli decrease under compression resulting in a positive entropy. The melting point of the triangular lattice is about $10^{-2}(\kappa d_0^2/k)$,[14] and so the vibrational entropy multiplied by the temperature ($\simeq 0.003\kappa d_0^2$) is always small compared with the strain energy ($\simeq 0.2\kappa d_0^2$).

TABLE IV. Entropies of dislocation pairs. The entropy changes due to the presence of a single pair of edge dislocations, a distance r apart, computed at a density $\rho = 1.1$ using Eq. (6) of the text.

r/b	ϵ	N_2	$\Delta S_{\rm vib}/k$
2	0.10	75	0.1800
		192	0.1795
	0.20	75	0.1972
4	0.00	192	0.2280
	0.10	75	0.2627
		192	0.2672
	0.20	75	0.2921
6	0.00	192	0.2563
8	0.00	192	0.2729
10	0.00	192	0.2849

D. Stresses of dislocations in finite-size crystals

A dislocation produces a macroscopic displacement, proportional to the Burgers vector and the distance moved.[8,19] For a pair of dislocations, in a crystal with fixed periodic boundary conditions, this results in a shear strain, $\epsilon_{xy} = br/V$—in our calculations we use the unsymmetrized strain tensor $\overleftrightarrow{\epsilon} = \vec{\nabla}\,\vec{u}$, where $\vec{u}$ is the displacement vector—and for the triplets a dilation, $\epsilon_{xx} = \epsilon_{yy} = \sqrt{3}br/2V$, where $V = (\sqrt{3}/2)Nb^2$. This dilatation corresponds, exactly, to the number of atoms removed. Thus elastic theory predicts that there should be a shear stress for the pair arrangement, $\sigma_{xy} = (2\eta r/\sqrt{3}bN)$, with all other stresses being zero. These predictions are compared with results

TABLE V. Stresses of dislocation pairs and triplets. The stresses for each arrangement of dislocations were fitted by polynomials in $1/N$. The best values for the linear $(1/N)$ deviations of the stresses from the infinite-system limit are given below, together with the predictions of elastic theory.

		Atomic simulation			Elastic theory		
	r/b	$N\sigma_{xx}/\kappa$	$N\sigma_{yy}/\kappa$	$N\sigma_{xy}/\kappa$	$N\sigma_{xx}/\kappa$	$N\sigma_{yy}/\kappa$	$N\sigma_{xy}/\kappa$
Pairs	6	1.21	0.12	2.55	0	0	2.56
	8	1.32	0.13	3.40	0	0	3.41
	10	1.4	0.1	4.26	0	0	4.27
	12	1.4	0.1	5.10	0	0	5.12
Triplets	4	1.39	1.39	0	0	0	0
	6	1.51	1.51	0	0	0	0
	8	1.6	1.6	0	0	0	0

from the atomic simulations in Table V. The shear stresses obtained from the atomic calculations are in essentially exact agreement with elastic theory. The reasonably constant values of $N\sigma_{xx}$ and $N\sigma_{yy}$ indicate the presence of a core stress, proportional to b^2/N, in the range $0.7 < N\sigma_{bb}/\kappa < 1.0$. These core stresses, which are absent from the elastic theory make only a small contribution to the energy of dislocations in finite-sized crystals.

E. Energies of dislocations in finite-size crystals

Elastic theory can be used to calculate the energy of dislocations in finite-size periodic crystals.[8]

TABLE VI. Dislocation core energies. The core energy in an arrangement of n dislocations is given by $E_c = (E_n - E_{LS} - E_s)/n$. The energy E_n is obtained from atomic calculations (Table I); E_{LS} is the sum of the pair energies [Eq. (2)] over all periodic images (Appendix); and E_s is the shear energy [Eq. (7)].

r/b	N_2	$E_{LS}/\kappa d_0^2$	$E_c/\kappa d_0^2$	N_3	$E_{LS}/\kappa d_0^2$	$E_c/\kappa d_0^2$
4	192	0.025 027	0.086 692	184	0.169 239	0.086 372
				292	0.186 215	0.087 822
				424	0.195 245	0.088 401
				964	0.206 401	0.088 891
				∞		0.089 1
6	192	0.053 798	0.086 833	180	0.155 962	0.080 917
	243	0.054 198	0.086 795			
	300	0.054 751	0.086 752	288	0.195 614	0.084 606
	432	0.055 851	0.086 674	420	0.216 643	0.086 177
	972	0.057 924	0.086 548	960	0.242 137	0.087 525
	∞		0.086 4	∞		0.088
8	192	0.076 808	0.086 549	176	0.105 611	0.075 910
	243	0.075 879	0.086 582			
	300	0.075 612	0.086 599	284	0.174 504	0.080 998
	432	0.076 067	0.086 586	416	0.213 076	0.083 863
	972	0.078 409	0.086 491	956	0.259 973	0.086 581
	∞		0.086 4	∞		0.088
10	192	0.096 049	0.086 491			
	243	0.095 041	0.086 383			
	300	0.093 771	0.086 384			
	432	0.092 621	0.086 432			
	972	0.094 041	0.086 412			
	∞		0.086 4			
12	300	0.109 719	0.086 313			
	432	0.107 631	0.086 279			
	972	0.106 891	0.086 333			
	∞		0.086 4			

These energies are useful in attempting to understand, quantitatively, the role of dislocations in computer simulations of plastic flow in small crystals. The periodic energy calculations may also lead to more accurate core energies by estimating the number dependence of the dislocation interaction energies. For a crystal with periodic boundaries, the energy sum in Eq. (2) must include all periodic images. We use the Ewald method,[8] described in the Appendix, to evaluate these lattice sums. In addition, there is typically an energy arising from the macroscopic deformations caused by the dislocations. The energy due to the average shear stress caused by a pair of dislocations is

$$E_s = \eta r^2/\sqrt{3}N \ . \tag{7}$$

When atoms are removed to accommodate dislocations, the density changes. Thus, for the triangular arrangement, there is an ambiguity in assigning the thermodynamic state. We use the density of the crystal with dislocations (i.e., $\rho = 1.1$) to calculate the elastic constants. The Burgers vector is chosen so that the periodic repeat distance is an integer multiple of it. Different choices do not affect the extrapolated values of the core energy, but change the core energies for small crystals by about $0.005\kappa d_0^2$. The results are collected in Table VI.

For the pair arrangement, the core energies are spread over a narrow range of $0.0005\kappa d_0^2$. The small number dependence of these core energies shows that elastic theory, adapted to finite-size periodic crystals, works remarkably well, even when the dislocation separation is comparable to the periodic repeat distance. The lattice sum of the dislocation energy $E_{\rm LS}$ is not a simple function of the number of atoms in the crystal. In particular, $(\partial E_{\rm LS}/\partial N)_r$ changes sign when the dislocation separation is half the repeat distance. This explains the small inconsistency when $r = 12b$ in the energy obtained by direct extrapolation of the simulation results. For the triangular arrangement, there is a significant number dependence in the core energies associated with the slightly arbitrary thermodynamic state. The discrepancies are an order of magnitude smaller than those reported by Fisher *et al.*[8] for the two-dimensional electron crystal.

The core energies for the various size systems have been extrapolated to the large-N limit. For all the pairs, the extrapolated core energy is $0.0864\kappa d_0^2$. For the triplets it is about $0.088\kappa d_0^2$. This discrepancy could be due to nonlinear elastic effects. In particular the dislocation separation in the triangular arrangement is not likely to be an integer multiple of the Burgers vector. The difference in core energies could be explained by shifts in the location of the dislocations of about 0.1 b.

ACKNOWLEDGMENT

This work was supported in the Department of Applied Science by the United States Army Research Office, Research Triangle Park, North Carolina, and by the U. S. Department of Energy at Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

APPENDIX: DISLOCATION INTERACTION ENERGIES IN PERIODIC CRYSTALS

The interaction energy, per unit cell, of a periodic array of n dislocations, is

$$\begin{aligned} E_{\rm LS} &= \sum_{i>j}^{n} \sum_{\vec{\rm R}} E_D(\vec{\rm b}_i, \vec{\rm b}_j; \vec{\rm R} - \vec{\rm r}_{ij}) \\ &\quad + \tfrac{1}{2} \sum_{i}^{n} \sum_{R \neq 0} E_D(\vec{\rm b}_i, \vec{\rm b}_i; \vec{\rm R}) \ , \\ E_D(\vec{\rm b}_1, \vec{\rm b}_2; \vec{\rm r}) &= D \left[-(\vec{\rm b}_1 \cdot \vec{\rm b}_2) \ln(r/b) + \frac{(\vec{\rm b}_1 \cdot \vec{\rm r})(\vec{\rm b}_2 \cdot \vec{\rm r})}{r^2} \right] . \end{aligned} \tag{A1}$$

The sum over $\vec{\rm R}$ includes vectors linking lattice points in the periodic hexagonal array. This set of vectors can be generated by writing $\vec{\rm R} = n_1 \vec{\rm L}_1 + n_2 \vec{\rm L}_2$ and summing over all integer values of n_1 and n_2. The vectors $\vec{\rm L}_1$ and $\vec{\rm L}_2$ are inclined at an angle of 60° to each other and are of length $\sqrt{3}L$, where L is the side length of the hexagon. These vectors are perpendicular bisectors of the sides of the hexagon.

The series can be summed by decomposing the interaction energy E_D into a short-range $E_<$ and a long-range $E_>$ part. We use the same choice for $E_<$ as Ref. 8, namely,

$$E_< = D \left[\tfrac{1}{2}(\vec{\rm b}_1 \cdot \vec{\rm b}_2)[E_1(\alpha r^2) + \ln(\alpha b^2) + \gamma] + \frac{(\vec{\rm b}_1 \cdot \vec{\rm r})(\vec{\rm b}_2 \cdot \vec{\rm r})}{r^2} e^{-\alpha r^2} \right] , \tag{A2}$$

where $E_1(x) = \int_x^\infty (e^{-t}/t)\,dt$ is the exponential integral function, and γ is Euler's constant. The lattice sum of $E_<$ is rapidly convergent, if α is of order L^{-2}, and is summed directly. The long-range part is Fourier transformed and summed in reciprocal space.

The reciprocal lattice is the set of vectors $\vec{k}=n_1\vec{k}_1+n_2\vec{k}_2$, where $\vec{k}_1$ and $\vec{k}_2$ are vectors of length $4\pi/3L$, inclined at an angle of 120° to each other. The sum of $E_>$ can be written as

$$\sum_{\vec{R}} E_>(\vec{R}-\vec{r})=(2\sqrt{3}/9L^2)\sum_{\vec{k}\neq 0} e^{-i\vec{k}\cdot\vec{r}}E_>(\vec{k}) , \tag{A3}$$

where $E_>(\vec{k})$ is the Fourier transform of $E_>(\vec{r})$,

$$E_>(\vec{k})=\int e^{-i\vec{k}\cdot\vec{r}}E_>(\vec{r})d\vec{r} . \tag{A4}$$

In Eq. (A3), a factor $(2/\sqrt{3})$ arises in transforming from oblique coordinates to the rectangular ones used in defining the Fourier transform [Eq. (A4)]. The terms with $k=0$ cancel out when summed over a number of dislocations with a total Burgers vector of zero.

The two-dimensional Fourier transform ("Fourier-Bessel transform"[20]) of $E_>$ can be written as

$$E_>(\vec{k})=D\left[\tfrac{1}{2}(\vec{b}_1\cdot\vec{b}_2)[g(k)+g_0(k)+g_2(k)] -\frac{(\vec{b}_1\cdot\vec{k})(\vec{b}_2\cdot\vec{k})}{k^2}g_2(k)\right] , \tag{A5}$$

where the scalar coefficients are integrals involving Bessel functions,

$$\begin{aligned} g(k)&=2\pi\int_0^\infty\{-[E_1(\alpha r^2)+\ln(\alpha r^2)+\gamma] \\ &\qquad\times J_0(kr)r\}dr , \\ g_n(k)&=2\pi\int_0^\infty(1-e^{-\alpha r^2})J_n(kr)r\,dr . \end{aligned} \tag{A6}$$

Using the series expansion for the exponential integral function,[21] we obtain an equation for $g(k)$, $\alpha(\partial g/\partial\alpha)=-g_0$. Although the integrands in Eq. (A6) diverge as $r\to\infty$, the integrals themselves are finite for nonzero k. Using the standard integrals tabulated in Ref. 22, we find that

$$\begin{aligned} g_0(k)&=I_0-(\pi/\alpha)e^{-k^2/4\alpha} , \\ g_2(k)&=(4\pi/k)\int_0^\infty(1-e^{-\alpha r^2})J_1(kr)dr \\ &\quad -g_0(k) \\ &=(4\pi/k^2)(1+k^2/4\alpha)e^{-k^2/4\alpha}-I_0 , \end{aligned} \tag{A7}$$

where all the diverging integrands are contained in the integral

$$I_0=2\pi\int_0^\infty J_0(kr)r\,dr=4\pi^2\delta(\vec{k}) . \tag{A8}$$

Thus collecting terms, we obtain for $E_>(\vec{k})$,

$$E_>(\vec{k})=(4\pi D/k^2)(e^{-k^2/4\alpha})\left[\vec{b}_1\cdot\vec{b}_2-\frac{(\vec{b}_1\cdot\vec{k})(\vec{b}_2\cdot\vec{k})}{k^2}[1+(k^2/4\alpha)]\right] . \tag{A9}$$

This is the same as the expression given in Ref. 8 for the case $\vec{b}_1=-\vec{b}_2$.

Useful checks of the analysis and the numerical procedure are that $E_{\rm LS}$ is independent of α and reflects the periodicity of the unit cell. If $r/L\ll 1$, $E_{\rm LS}$ can be approximated by Eq. (2).

---

[1] J. J. Gilman, *Micromechanics of Flow in Solids* (McGraw-Hill, New York, 1969).

[2] Y. M. Gupta, Ph.D. thesis, Washington State University, 1973 (unpublished).

[3] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Clarendon, Oxford, 1953); F. R. N. Nabarro, *Theory of Crystal Dislocations* (Clarendon, Oxford, 1967); *Dislocation Dynamics*, edited by A. R. Rosenfield, G. T. Hahn, A. L. Bement, and R. I. Jaffee (McGraw-Hill, New York, 1968); X. Markenscoff and R. J. Clifton, J. Mech. Phys. Solids 29, 253 (1981). For recent work, see *Dislocation Modelling of Physical Systems*, edited by M. F. Ashby, R. Bullough, and C. S. Hartley (Pergamon, New York, 1980).

[4] R. Bullough and V. K. Tewary, in *Dislocations in Solids*, edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1979), Vol. 2.

[5] A. A. Maradudin, J. Phys. Chem. Solids 9, 1 (1958); V. Celli and N. Flytzanis, J. Appl. Phys. 41, 4443 (1970); N. Flytzanis, V. Celli, and A. Nobile, *ibid.* 45, 5176 (1974); J. H. Weiner and M. Pear, *ibid.* 46, 2398 (1975).

[6] W. G. Hoover, N. E. Hoover, and W. C. Moss, J. Appl. Phys. 50, 829 (1979).

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

[8] D. S. Fisher, B. I. Halperin, and R. Morf, Phys. Rev. B 20, 4692 (1979).

[9] L. Davison and R. A. Graham, Phys. Rep. 55, 255 (1979).

[10] V. Y. Klimenko and A. N. Dremin, in *Detonatsiya Chernogolovka,* edited by O. N. Breusov *et al.* (Akad. Nauk., Moscow, 1978), p. 79. W. G. Hoover, Phys. Rev. Lett. 42, 1531 (1979); B. L. Holian, W. G. Hoover, B. Moran, and G. K. Straub, Phys. Rev. A 22, 2798 (1980). Note that the coefficient 1.864 on page 2806 is a misprint. The correct coefficient is 1.684.

[11] W. G. Hoover, A. J. C. Ladd, and B. Moran, Phys. Rev. Lett. 48, 1818 (1982). Replace the misprint, $\partial \dot{l}/\partial l$, on p. 1819 with $\partial \dot{p}/\partial p$.

[12] *Shock Waves and High Strain-Rate Phenomena in Metals,* edited by M. A. Meyers and L. E. Murr (Plenum, New York, 1981); *Shock Waves in Condensed Matter,* edited by W. J. Nellis, L. Seaman, and R. A. Graham (AIP, New York, 1981).

[13] D. C. Wallace, Phys. Rev. B 22, 1487 (1979); 24, 5607 (1981).

[14] See, for example, R. Bruinsma, B. I. Halperin, and A. Zippelius, Phys. Rev. B 25, 579 (1982).

[15] R. W. Werne and J. M. Kelly, Int. J. Eng. Sci. 16, 951 (1978).

[16] W. G. Hoover, A. J. C. Ladd, and N. E. Hoover, in *Interatomic Potentials and Crystalline Defects,* edited by J. K. Lee (Metallurgical Society, Warrendale, Penn., 1981); A. J. C. Ladd and W. G. Hoover, J. Chem. Phys. 74, 1337 (1981).

[17] W. G. Hoover, A. C. Hindmarsh, and B. L. Holian, J. Chem. Phys. 57, 1980 (1972).

[18] P. D. Crout, Trans. Am. Inst. Elec. Eng. 60, 1235 (1941).

[19] D. R. Nelson and B. I. Halperin, Phys. Rev. B19, 2457 (1979).

[20] H. Margenau and G. M. Murphy, *The Mathematics of Physics and Chemistry,* 2nd ed. (Van Nostrand, New York, 1956).

[21] *Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Natl. Bur. Stand., Washington, D. C., 1972).

[22] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965).