The dynamics of free, straight dislocation pairs. I. Screw dislocations

R. Eykholt
Department of Physics, Colorado State University, Fort Collins, Colorado 80523 and Los Alamos National Laboratory, Los Alamos, New Mexico 87545

S. A. Trugman
Los Alamos National Laboratory, Los Alamos, New Mexico 87545

D. J. Solovitz
Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan 48109-2136 and Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 31 October 1988; accepted for publication 1 February 1989)

Analytic expressions are derived for the motion of a pair of interacting, straight, parallel (or antiparallel) screw dislocations in an applied stress field. Analysis of the equations of motion of the dislocations shows that, under most circumstances, the velocity of a dislocation is proportional to the driving force (i.e., the motion is overdamped), and, in this limit, the results are exact. However, when the two dislocations are very close together, inertial terms begin to play a role, and the resultant "finite-mass" corrections are treated perturbatively. For the case of antiparallel screw dislocations, a capture cross section exists and is given by the product of the shear modulus and the Burgers vector over the applied stress. Based on these results, a simple statistical analysis of the motion of a large number of screw dislocations is presented.

I. INTRODUCTION

The role of dislocations as the mediators of deformations in metals is both well known and ubiquitous. In addition to controlling plastic deformation, dislocations play a major role in determining the fracture behavior of a wide variety of materials. In both of these cases, material properties are determined by the motion of large numbers of interacting dislocations. (Typical dislocation densities in metals lie in the range 10^8–10^{12} dislocations/cm^2.) The difficulty inherent in the analytical treatment of such large densities of defects is compounded by the relatively slow rate of decay of their stress fields with separation (i.e., $\sigma \sim 1/r$). In contrast, the properties of individual dislocations are rather well understood.[1] The stress field about an arbitrarily oriented dislocation in an anisotropic material is now well established.[2] Similarly, the dynamical properties of individual dislocations have received considerable attention.[3] However, little progress has been made in employing the well-established properties of individual dislocations in a description of the dynamical behavior of collections of dislocations.

Previous experience with dynamical systems has shown that, while true many-body problems are, inherently, extremely difficult, two-body problems are often tractable. In this same spirit, we attempt to solve for the motion of a pair of dislocations. While, admittedly, such solutions do not constitute tremendous progress toward a description of the collective motion of realistically large numbers of dislocations, they do constitute a first step towards solving the problem of multidislocation dynamics. Furthermore, such solutions are directly applicable in the low-density limit. In addition, computer simulation techniques have recently been developed which numerically simulate the motion of many dislocations under a restricted set of assumptions.[4,5] One of the difficulties encountered in such approaches occurs when the separation between a pair of dislocations becomes much smaller than the mean interdislocation spacing. In such cases, proper integration of the equations of motion requires formidably short time steps. However, an analytical description of dislocation trajectories of unusually closely spaced pairs helps alleviate this problem. Such approaches are commonly used in studying the molecular dynamics of hard-sphere systems.

In this paper, we derive analytic expressions for the motion of a pair of screw dislocations in an infinite body in two spatial dimensions (i.e., parallel or antiparallel, straight dislocations). In Sec. II, we derive an equation of motion appropriate for a pair of straight dislocations interacting with each other and with an externally applied stress field (which can include the average field of other dislocations). The trajectory of the center of mass of a pair of parallel or antiparallel screw dislocations is the subject of Sec. III. Sections IV and V present exact solutions for the relative motion of a pair of parallel or antiparallel screw dislocations in the overdamped limit, both with and without the presence of an external stress. The effects of relaxing the constraint of overdamping are treated perturbatively. Finally, a simple, statistical application of these results to the many-body problem is presented. Similar results for edge dislocations are presented in a separate publication.[6]

II. EQUATION OF MOTION

When a dislocation moves through a crystalline lattice, there is movement of both the atoms in the core region of the dislocation and those far away. The faster the dislocation moves, the more kinetic energy is imparted to these atoms. Neglecting the relatively small contribution of the dislocation core, Eshelby[7] and others[8,9] have shown that this kinetic energy scales as the square of the dislocation velocity (for the velocity v much less than the transverse sound velocity

 0021-8979/89/114198-06$02.40

c_t). Therefore, the dislocation has an effective mass m^*, which is given by

$$E_{\rm kin} = \frac{1}{2} m^* v^2 = \frac{\mu b^2}{8\pi}\left(\frac{v^2}{c_t^2}\right)\ln\left(\frac{R_c}{r_c}\right),$$

$$m^* = \frac{\mu b^2}{4\pi c_t^2}\ln\left(\frac{R_c}{r_c}\right), \qquad (2)$$

where μ is the shear modulus, b is the magnitude of the Burgers vector, and R_c and r_c are the outer and inner cutoff radii, respectively. Since a moving dislocation has mass, it carries momentum, and, hence, should behave as a Newtonian particle: $m^*\ddot{\mathbf{x}} = \mathbf{F}$, where the dots indicate differentiation with respect to time, $\mathbf{x}$ is the vector position of the dislocation, and $\mathbf{F}$ is the force on the dislocation.

Since dislocations in metals exit on a lattice (and, therefore, have cores) instead of in a true continuum, a moving dislocation radiates phonons. Such effects are well known for dislocations, as well as for essentially all defects moving through a lattice. Therefore, the movement of the dislocation dissipates energy, and its motion is nonconservative. In addition to the aforementioned phonon-emission/core-dissipation mechanism, a number of other dissipation mechanisms are known to exist (e.g., thermal-phonon scattering, electron scattering, etc.). In metals, the scattering of thermal phonons by the moving dislocations is the dominant dissipation mechanism, except at very low temperatures.

The presence of dissipation modifies the equation of motion for the dislocation:

$$\mathbf{F} = m^*\ddot{\mathbf{x}} + \gamma\,\dot{\mathbf{x}}\,, \qquad (3)$$

where γ is the damping coefficient (see Ref. 10 for a discussion of this damping term). For the case of thermal-phonon scattering,[10] we have

$$\gamma = (\mu b/c_t)\, g(T/\Theta)\,, \qquad (4)$$

where Θ is the Debye temperature, and the function $g(T/\Theta)$ varies from approximately 10^{-3} at $T = 0.1\Theta$ to 2×10^{-2} at $T = \Theta$. While we ignore crystalline anisotropy in the present analysis, we note that, in general, both the dislocation mass m^* and the damping coefficient γ are second-rank tensors instead of scalars (i.e., we have taken m^* and γ to be multiples of the identity matrix).

For a pair of screw dislocations, the force in Eq. (3) has contributions from both the externally applied stress $\boldsymbol{\sigma}_A$ and that due to the interaction between the two dislocations. The force on dislocation 1 due to dislocation 2 (in the coordinate system of Fig. 1) may be written as

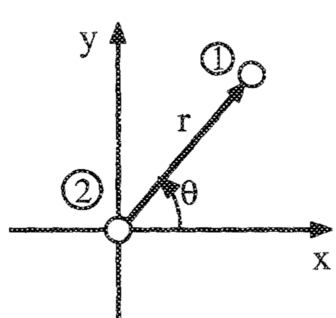

FIG. 1. Illustration of the coordinate system used for the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. The Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ are each either into or out of the paper.

$$F_{12} = \pm(\mu b_1 b_2/2\pi r^2)(\hat{\mathbf{x}}x + \hat{\mathbf{y}}y)$$

$$= \pm(\mu b_1 b_2/2\pi r)\hat{\mathbf{r}}\,, \qquad (5)$$

where a caret (^) indicates a unit vector, and the upper and lower signs are for parallel and antiparallel screw dislocations, respectively. Equation (5) may be derived from the stress field of dislocation 2 at the position of dislocation 1 and the Peach–Kohler formula.[11]

The dissipative term in the equation of motion (3) may be expected to dominate the Newtonian or inertial term as long as the dislocation is not accelerating too quickly. For the case of two attracting (antiparallel) screw dislocations, we can estimate how close the two dislocations must get for the inertial term to become important. Setting m^* to zero and inserting Eq. (5) into Eq. (3) we find

$$-(\mu b^2/2\pi r) = \gamma\dot{r}\,. \qquad (6)$$

Differentiating Eq. (6) with respect to time and rearranging terms yields

$$\ddot{r}/\dot{r} = \mu b^2/2\pi\gamma r^2\,. \qquad (7)$$

In order for the inertial term to dominate the dissipative term, we must have $m^*\ddot{r} > \gamma\dot{r}$ ($\ddot{r}/\dot{r} > \gamma/m^*$). Inserting Eq. (7) into this inequality shows that the inertial term is important only for

$$r < (\mu m^*/2\pi)^{1/2}(b/\gamma) \sim 50b\,. \qquad (8)$$

Therefore, for dislocation separations greater than about 100 Å, the motion of the dislocations is overdamped, and the inertial term is negligible. Under these conditions, we write $\mathbf{F} \simeq \gamma\dot{\mathbf{x}}$, and the inertial term may be treated as a perturbation.

III. CENTER-OF-MASS COORDINATES

We consider two screw dislocations of effective mass m^*, with Burgers vectors of equal magnitude b, which are either parallel ($\epsilon = 1$) or antiparallel ($\epsilon = -1$). The equations of motion (3) for dislocations 1 and 2 are

$$m^*\ddot{\mathbf{r}}_1 = \frac{\epsilon\mu b^2}{2\pi}\frac{(\mathbf{r}_1 - \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|^2} + \mathbf{F}_A - \gamma\,\dot{\mathbf{r}}_1\,, \qquad (9a)$$

$$m^*\ddot{\mathbf{r}}_2 = -\frac{\epsilon\mu b^2}{2\pi}\frac{(\mathbf{r}_1 - \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|^2} + \epsilon\mathbf{F}_A - \gamma\,\dot{\mathbf{r}}_2\,, \qquad (9b)$$

where $\mathbf{F}_A = \underline{\sigma}_A \cdot \mathbf{b}_1$ is the applied, external force. Here, we have taken the system to be infinite in extent, and we have neglected any Peierls stress, which is valid if the total stress is not too small. We now switch to center-of-mass and relative coordinates $\mathbf{R} = (1/2)(\mathbf{r}_1 + \mathbf{r}_2)$ and $\mathbf{r} = (\mathbf{r}_1 - \mathbf{r}_2)$, respectivley, in terms of which Eqs. (9) become

$$m^*\ddot{\mathbf{R}} = \tfrac{1}{2}(1+\epsilon)\mathbf{F}_A - \gamma\dot{\mathbf{R}}, \qquad (10a)$$

$$m^*\ddot{\mathbf{r}} = (\epsilon\mu b^2/\pi r^2)\mathbf{r} + (1-\epsilon)\mathbf{F}_A - \gamma\,\dot{\mathbf{r}}\,. \qquad (10b)$$

The motion $\mathbf{R}(t)$ of the center of mass may be solved for by direct integration of Eq. (10a). One integration yields

$$m^*(\dot{\mathbf{R}} - \mathbf{V}_0) + \gamma(\mathbf{R} - \mathbf{R}_0) + \tfrac{1}{2}(1+\epsilon)\mathbf{F}_A t = 0\,, \qquad (11)$$

where $\mathbf{R}_0 = \mathbf{R}(t=0)$ and $\mathbf{V}_0 = \dot{\mathbf{R}}(t=0)$. Multiplying though by $e^{\gamma t/m^*}$ and integrating once more yields

$$\mathbf{R}=\mathbf{R}_0+\left(\frac{1+\epsilon}{2\gamma}\right)\mathbf{F}_A t+\frac{m^*}{\gamma}\left[\mathbf{V}_0-\left(\frac{1+\epsilon}{2\gamma}\right)\mathbf{F}_A\right]$$
$$\times(1-e^{-\gamma t/m^*}). \tag{12}$$

In the overdamped limit (i.e., $m^*\to 0$), this reduces to

$$\mathbf{R}=\mathbf{R}_0+\left(\frac{1+\epsilon}{2\gamma}\right)\mathbf{F}_A t. \tag{13}$$

For the case of parallel screws ($\epsilon=1$), this shows that the center of mass translates with a constant velocity $\mathbf{F}_A/\gamma$. However, when the screws are antiparallel ($\epsilon=-1$), the center of mass is stationary.

It is important to note that this exact solution illustrates the fact that the effects of the finite effective mass of the dislocations decay away exponentially fast with time constant $\tau=m^*/\gamma$. Employing Eqs. (2) and (4) and choosing $c_t=2.3\times10^3$ m/s, $r_c=b=2.5\times10^{-10}$ m, and $R_c=5\times10^{-7}$ m yields $\tau=3.3\times10^{-12}$ s. This again suggests that the overdamped limit is appropriate.

IV. PARALLEL SCREWS

When the screw dislocations are parallel (i.e., identical line directions and Burgers vectors), the equation of motion [Eq. (10b)] for the relative coordinate reduces to

$$m^*\ddot{\mathbf{r}}=(\mu b^2/\pi r^2)\mathbf{r}-\gamma\dot{\mathbf{r}}. \tag{14}$$

This equation is independent of the applied force or stress, which only translates the center of mass. Noting that

$$\dot{\mathbf{r}}=\hat{\mathbf{r}}\dot{r}+\hat{\boldsymbol{\theta}}r\dot{\theta}$$

and

$$\ddot{\mathbf{r}}=\hat{\mathbf{r}}(\ddot{r}-r\dot{\theta}^2)+\hat{\boldsymbol{\theta}}(r\ddot{\theta}+2\dot{r}\dot{\theta}),$$

Eq. (14) may be rewritten as

$$m^*(\ddot{r}-r\dot{\theta}^2)+\gamma\dot{r}-(\mu b^2/\pi r)=0, \tag{15a}$$
$$m^*(r\ddot{\theta}+2\dot{r}\dot{\theta})+\gamma r\dot{\theta}=0. \tag{15b}$$

In the overdamped limit ($m^*=0$), these equations may readily be integrated to yield

$$\theta=\theta_0, \tag{16a}$$
$$r=[r_0^2+(2\mu b^2 t/\pi\gamma)]^{1/2}, \tag{16b}$$

where $\theta_0=\theta(t=0)$ and $r_0=r(t=0)$.

We obtain finite-effective-mass corrections to Eqs. (16) by returning to the original equation of motion for θ [Eq. (15b)]. After multiplying by $r^2e^{\gamma t/m^*}$, this equation may be integrated to yield

$$\dot{\theta}=\omega_0(r_0/r)^2e^{-\gamma t/m^*}, \tag{17}$$

where $\omega_0=\dot{\theta}(t=0)$. In this equation, note that r is a function of time. Inserting the overdamped solution for $r(t)$ [Eq. (16b)] into Eq. (17) and integrating with respect to time yields the lowest-order, finite-effective-mass correction to Eq. (16a):

$$\theta=\theta_0+\frac{\pi\gamma r_0^2\omega_0}{2\mu b^2}e^{\pi\gamma^2r_0^2/2\mu b^2m^*}$$
$$\times\left[E_1\left(\frac{\pi\gamma^2r_0^2}{2\mu b^2m^*}\right)-E_1\left(\frac{\pi\gamma^2r_0}{2\mu b^2m^*}+\frac{\gamma t}{m^*}\right)\right], \tag{18}$$

where $E_1(z)$ is related to the exponential-integral function and is defined as

$$E_1(z)=\int_z^\infty\frac{dx}{x}e^{-x}. \tag{19}$$

Expanding this to lowest order in m^* yields

$$\theta=\theta_0+\frac{m^*\omega_0}{\gamma}\left[1-\left(1+\frac{2\mu b^2t}{\pi\gamma r_0^2}\right)^{-1}e^{-\gamma t/m^*}\right]. \tag{20}$$

As for the center-of-mass coordinate, the finite-effective-mass contribution decays exponentially with time constants m^*/γ. In the limit as $t\to\infty$, this becomes

$$\theta=\theta_0+(m^*\omega_0/\gamma). \tag{21}$$

Thus, θ changes very little over the entire trajectory.

The lowest-order, finite-m^* correction to $r(t)$ [Eq. (16b)] is found by inserting this overdamped solution into the inertial term of the original equation of motion (15a). Retaining only those lowest-order terms in m^*, we find

$$r=\left(r_0^2+\frac{2\mu b^2t}{\pi\gamma}\right)^{1/2}+\frac{\mu b^2m^*}{2\pi\gamma^2}\left(r_0^2+\frac{2\mu b^2t}{\pi\gamma}\right)^{-1/2}$$
$$\times\ln\left(1+\frac{2\mu b^2t}{\pi\gamma r_0^2}\right). \tag{22}$$

Thus, the separation between the two parallel screws grows as $t^{1/2}$ at long times. On the other hand, the finite-m^* correction decays as $t^{-1/2}\ln t$ at long times.

The finite-effective-mass corrections derived above are valid for

$$r_0^2\gg\mu b^2m^*/2\pi e\gamma^2, \tag{23a}$$
$$\omega_0\ll 2\pi\gamma/m^*, \tag{23b}$$

where e is the base of the natural logarithm. These conditions guarantee that the acceleration of the dislocations at $t=0$ (and, thus, at all successive times) does not violate the assumption of the dominance of dissipation over inertia. Improved estimates of the finite-effective-mass correction can be obtained by inserting the corrected $r(t)$ [Eq. (22)] into Eqs. (15a) and (17). Arbitrarily high accuracy may be obtained by continued substitution of the increasingly accurate solutions for $r(t)$ into the exact expressions.

V. ANTIPARALLEL SCREWS

Antiparallel screw dislocations (i.e., the same line direction, but opposite Burgers vectors) move in opposite directions when subjected to the same externally applied stress. In the overdamped limit ($m^*=0$), this results in no net motion of the center of mass of the pair [Eq. (13)]. The relative coordinate, on the other hand, evolves with time as given by Eq. (10b):

$$m^*\ddot{\mathbf{r}}=-(\mu b^2/\pi r^2)\mathbf{r}+2\mathbf{F}_A-\gamma\dot{\mathbf{r}}. \tag{24}$$

In the overdamped limit, this reduces to

$$\gamma\dot{r}=-(\mu b^2/\pi r)-2F_A\cos\theta, \tag{25a}$$
$$\gamma r\dot{\theta}=2F_A\sin\theta, \tag{25b}$$

where we have chosen the x axis to lie along $-\mathbf{F}_A$. The coordinate $\mathbf{r}$ gives the position of dislocation 1 relative to dislocation 2, as illustrated in Fig. 1. Cross multiplying Eqs. (25a) and (25b) and integrating yields

$$(\mu b^2/2\pi)\theta + F_A r \sin\theta = C, \qquad (26)$$

where C is a constant which is determined by the initial conditions: namely,

$$C = (\mu b^2/2\pi)\theta(t=0) + F_A r(t=0)\sin\theta(t=0)$$
$$= (\mu b^2/2\pi)\theta_0 + F_A r_0 \sin\theta_0 .$$

Equation (26) gives the path along which dislocation 1 travels. It is convenient to replace r by $y = r\sin\theta$, in which case, Eq. (26) becomes

$$y = (1/F_A)[C - (\mu b^2/2\pi)\theta], \qquad (27)$$

with $-\pi \leqslant \theta \leqslant \pi$.

A family of trajectories corresponding to different choices of $C = (\mu b^2/2\pi)\theta_0 + F_A y_0$ are shown in Fig. 2. Since no trajectories cross the x axis, and the trajectories are symmetric with respect to the x axis, we consider only the case $y > 0$. As $t \to -\infty$, we have $\theta \to 0$ and $y \to d = C/F_A$, which is the impact parameter with which dislocation 1 approaches dislocation 2. In terms of this impact parameter, Eq. (27) becomes

$$y = d - (\mu b^2/2\pi F_A)\,\theta. \qquad (28)$$

If $d > \mu b^2/2F_A$, dislocation 1 approaches from the right (Fig. 2) and exits to the left at

$$d' = y(t=\infty) = d - \mu b^2/2F_A .$$

Note that the interaction of the two dislocations will always reduce the height of the trajectory by the same amount $d^* = \mu b^2/2F_A$ for any choice of $d > d^*$. For $d < d^*$, dislocation 1 approaches from the right and ends up at $y = 0$ for $\theta = \theta^* = \pi d/d^*$. In other words, dislocations 1 and 2 meet and annihilate if the impact parameter falls within the window $-d^* < d < d^*$. In the special case of $d = d^*$, dislocation 1 approaches a stagnation point at $y = 0$, $x = -d^*/\pi$.

The velocity of dislocation 1 along its trajectory may be calculated as

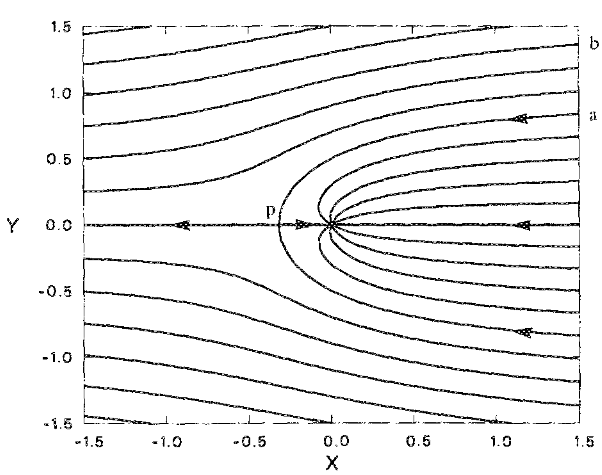

FIG. 2. Relative motion of two antiparallel screw dislocations in the overdamped limit ($m^* = 0$) in the presence of an external force $\mathbf{F}_A = -\hat{\mathbf{x}}F_A$. Trajectory a, whose initial, asymptotic approach is along $y = d^* = \mu b^2/2F_A$, approaches a stagnation point p as $t \to \infty$. A trajectory b which approaches along $y = d > d^*$ exits along $y = d - d^*$, with the drop d^* being independent of the initial approach d. All trajectories which approach along $y = d < d^*$ end up at the origin, resulting in the annihilation of the two dislocations. The coordinates x and y are plotted in units of d^*.

$$v = (\dot r^2 + r^2\dot\theta^2)^{1/2}$$
$$= \frac{2F_A}{\gamma}\left(1 + \frac{2\mu b^2 \sin\theta\cos\theta}{2\pi d F_A - \mu b^2\theta} + \frac{\mu^2 b^4 \sin^2\theta}{(2\pi d F_A - \mu b^2\theta)^2}\right)^{1/2}. \qquad (29)$$

For $d > d^*$, dislocation 1 approaches from $x = \infty$ with an asymptotic velocity $v = 2F_A/\gamma$, speeds up, slows down again, and finally leaves with the same asymptotic velocity. For $d < d^*$, dislocation 1 approaches with the asymptotic velocity $v = 2F_A/\gamma$, speeds up, and is captured by dislocation 2 with infinite velocity, approaching from the angle θ^*. In real solids, however, dislocation velocities are limited to the shear-wave velocity. Finally, for $d = \mu b^2/2F_A$, dislocation 1 approaches with the asymptotic velocity $v = 2F_A/\gamma$, speeds up, and then slows down and approaches the stagnation point with vanishing velocity.

An exact solution for the time dependence of the motion of the antiparallel screws is obtained by inserting Eq. (26) into Eq. (25b) (with $C = dF_A$) and integrating once with respect to time, which yields

$$t = \frac{\gamma}{4\pi F_A^2}\Big[(2\pi d F_A - \mu b^2\theta_0)\cot\theta_0$$
$$- (2\pi d F_A - \mu b^2\theta)\cot\theta - \mu b^2 \ln\left(\frac{\sin\theta}{\sin\theta_0}\right)\Big]. \qquad (30)$$

Unfortunately, Eq. (30) cannot be analytically inverted to yield $\theta(t)$. However, one can directly find the time corresponding to any value of θ. Similarly, one finds $r(\theta)$ and, indirectly, $r(t)$ by using Eq. (26) to write

$$r = (2\pi d F_A - \pi b^2\theta)/(2\pi F_A \sin\theta).$$

For $d < d^*$, we can find the time required for the pair of antiparallel screws to annihilate by calculating the time required for θ to go from θ_0 to $\theta^* = 2\pi d F_A/\pi b^2$ (see above). Inserting $\theta = \theta^*$ into Eq. (30) yields the capture time

$$\tau = \frac{\gamma}{4\pi F_A^2}\Big[(2\pi d F_A - \mu b^2\theta_0)\cot\theta_0$$
$$- \mu b^2 \ln\left(\frac{\sin(2\pi d F_A/\mu b^2)}{\sin\theta_0}\right)\Big]. \qquad (31)$$

τ decreases with increasing F_A and with increasing θ_0 for $\theta_0 < \theta^*$.

While it is not very illuminating to solve perturbatively for the trajectories of antiparallel screw dislocations with finite effective masses under the influence of an applied, external force, significant progress is possible in the zero-force limit. In this limit, Eq. (24) reduces to

$$m^*(\ddot r - r\dot\theta^2) + \gamma\dot r + (\mu b^2/\pi r) = 0, \qquad (32a)$$
$$m^*(r\ddot\theta + 2\dot r\dot\theta) + \gamma r\dot\theta = 0. \qquad (32b)$$

Equation (32b) is identical to Eq. (15b) and, hence, is solved in the same way. Similarly, apart from the sign of the $1/r$ term, Eq. (32a) is identical to Eq. (15a). Thus, proceeding as in Sec. IV, for $m^* = 0$, we find

$$\theta = \theta_0, \qquad (33a)$$
$$r = [r_0^2 - (2\mu b^2 t/\pi\gamma)]^{1/2}. \qquad (33b)$$

Setting $r = 0$ yields the capture time $\tau = \pi\gamma r_0^2/2\mu b^2$. Note that, in the absence of an applied force, a pair of antiparallel screws will eventually annihilate, regardless of their initial, relative positions (assuming, of course, that they are close enough together for their interactions to exceed any Peierls stress). The finite-m^* corrections are now calculated perturbatively as in Sec. IV to yield

$$r = r_0\left(1-\frac{t}{\tau}\right)^{1/2} - \frac{m^* r_0}{4\gamma\tau}\left(1-\frac{t}{\tau}\right)^{-1/2}\ln\left(1-\frac{t}{\tau}\right), \tag{34a}$$

$$\theta = \theta_0 + \frac{m^*\omega_0}{\gamma}\left[1-\left(1-\frac{t}{\tau}\right)^{-1} e^{-\gamma t/m^*}\right], \tag{34b}$$

where τ is the capture time. These expressions are valid for $\omega_0 \ll 2\pi\gamma/m^*$ and $\tau - t \gg m^*/4\gamma$.

VI. DISCUSSION

In the three previous sections, we have calculated the trajectories of a pair of parallel (or antiparallel) screw dislocations in the overdamped limit, which is most appropriate for dislocations in metals, ceramics, etc. Where possible, the assumption of massless (i.e., overdamped) dislocations has been relaxed. The motion of the dislocations has been calculated in the center-of-mass and relative coordinates. In order to relate these results to the laboratory frame one needs only to insert the expressions for the center-of-mass coordinate $\mathbf{R}$ and the relative coordinate $\mathbf{r}$ into the expressions

$$\mathbf{r}_1 = \mathbf{R} + \tfrac{1}{2}\mathbf{r}, \tag{35a}$$

$$\mathbf{r}_2 = \mathbf{R} - \tfrac{1}{2}\mathbf{r}. \tag{35b}$$

In addition to being an interesting exercise in dislocation theory and kinematics, we foresee two main applications of these results. The first, mentioned above, is in computer simulations of large numbers of dislocations. In this case, these solutions allow for the efficient integration of the equations of motion for the dislocations when two dislocations come within close proximity (relative to the mean dislocation spacing). The second is as a basis for the development of a statistical theory for the deformation of solids.

For the two-dimensional case considered here (i.e., straight screw dislocations), a number of interesting results may be derived in a relatively straightforward manner. First, however, we note that the equilibrium thermodynamics of such systems is well known as it appears in the literature of the Kosterlitz–Thouless transition (the interested reader is referred to Ref. 12 for an overview). Most of the interesting cases of dislocation dynamics are nonequilibrium, with the density of dislocations ρ evolving in time. Assuming a random spatial distribution of screw dislocations ($\rho_{\text{parallel}} = \rho_{\text{antiparallel}} = \rho$), we estimate the rate of change of the dislocation density as

$$\frac{\partial\rho}{\partial t} = -\sigma^* v \rho^2, \tag{36}$$

where σ^* is the applied-force-dependent capture cross section for a pair of dislocations, and v is the mean dislocation velocity ($v = F_A/\gamma$). Thus $\sigma^* v$ is the rate at which a dislocation sweeps area (and annihilates other dislocations). The ρ^2 dependence in Eq. (36) accounts for the fact that the dislocations annihilate in pairs.

In order to make use of Eq. (36), we use the results of the previous section to find

$$\sigma^* = 2d^* = \mu b^2/F_A. \tag{37}$$

Inserting Eq. (37) into Eq. (36) and using $v = F_A/\gamma$, we find

$$\frac{\partial\rho}{\partial t} = -\left(\frac{\mu b^2}{F_A}\right)\left(\frac{F_A}{\gamma}\right)\rho^2 = -(\mu b^2/\gamma)\rho^2. \tag{38}$$

Hence, the rate of annihilation is independent of the magnitude of the externally applied force or stress. Integration of (38) shows that the initial dislocation density ρ_0 decays as

$$\rho(t) = \frac{\rho_0}{1 + (\mu b^2/\gamma)\rho_0 t}. \tag{39}$$

While Eq. (39) describes the decay of an initial dislocation density, we should expect that additional dislocations are generated during deformation. In general, we may write

$$\frac{\partial\rho}{\partial t} = -\left(\frac{\mu b^2}{\gamma}\right)\rho^2 + \alpha\rho^\nu, \tag{40}$$

where α is a constant which may be a function of both the applied stress and the temperature and, ν is a constant which depends on the mechanism for dislocation generation.

For $\nu \neq 2$, Eq. (40) yields a finite equilibrium density ($\partial\rho/\partial t = 0$)

$$\rho^* = (\alpha\gamma/\mu b^2)^{1/(2-\nu)}. \tag{41}$$

The qualitative behavior of the dislocation density $\rho(t)$ may be found by examining Fig. 3. For $\nu < 2$, we see that, when $\rho < \rho^*$, we have $\partial\rho/\partial t > 0$ and ρ increases, while, for $\rho > \rho^*$, we have $\partial\rho/\partial t < 0$ and ρ decreases. Thus, for $\nu < 2$, the density $\rho(t)$ approaches the steady-state density ρ^*. On the other hand, for $\nu > 2$, a similar analysis shows that $\rho(t)$ evolves away from ρ^*, approaching zero for $\rho_0 < \rho^*$, or infinity for $\rho_0 > \rho^*$.

Equation (40) may also be solved analytically. Changing variables and integrating yields (for $\nu \neq 2$)

$$t = \frac{1-\lambda}{\alpha}\left(\frac{\alpha\gamma}{\mu b^2}\right)^\lambda \int_{\eta_0}^{\eta} z^{\lambda-1}(1-z)^{-1}\,dz, \tag{42}$$

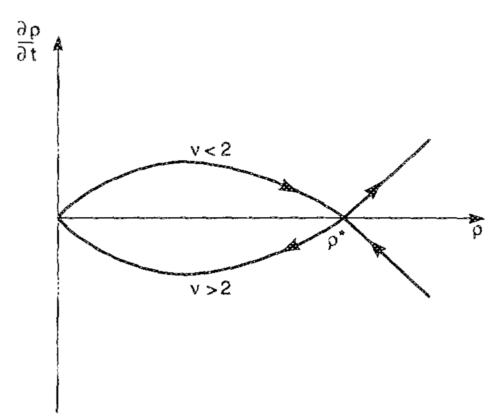

FIG. 3. To describe the time evolution of the density ρ of parallel and antiparallel dislocations, we plot $\partial\rho/\partial t$ vs ρ from Eq. (40). For $\nu < 2$, we see that, when $\rho < \rho^*$, we have $\partial\rho/\partial t > 0$ and ρ increases, while, for $\rho > \rho^*$, we have $\partial\rho/\partial t < 0$ and ρ decreases. In either case, $\rho(t)$ approaches the steady-state density ρ^*. On the other hand, for $\nu > 2$, $\rho(t)$ evolves away from ρ^*, approaching either $\rho = 0$ or $\rho = \infty$.

where $\lambda = (1-\nu)/(2-\nu), \eta = (\rho/\rho^*)^{2-\nu}$, and $\eta_0 = (\rho_0/\rho^*)^{2-\nu}$. For integer $\nu \neq 2$, this integral is an elementary function, and we have the following results [for $\nu = 2$, Eq. (40) may be solved directly]:

$\nu = 0$:

$$\rho(t) = \rho^* \left(\frac{\rho_0 \cosh \kappa t + \rho^* \sinh \kappa t}{\rho_0 \sinh \kappa t + \rho^* \cosh \kappa t} \right), \tag{43a}$$

$$\rho^* = (\alpha\gamma/\mu b^2)^{1/2},$$

$$\kappa = (\alpha\mu b^2/\gamma)^{1/2};$$

$\nu = 1$:

$$\rho(t) = \rho^* \{1 - [1 - (\rho^*/\rho_0]e^{-\alpha t}\}^{-1}, \tag{43b}$$

$$\rho^* = \alpha\gamma/\mu b^2;$$

$\nu = 2$:

$$\rho(t) = \rho_0 [1 + (\mu b^2/\gamma - \alpha)\rho_0 t]^{-1}. \tag{43c}$$

For integral $\nu > 2$, the integral yields t as an elementary function of ρ, but this cannot be analytically inverted to yield $\rho(t)$. Similarly, for nonintegral ν, the integral can be expressed in terms of incomplete beta functions, but this expression also cannot be analytically inverted to yield $\rho(t)$.

While such results do provide information about the evolution of the dislocation density, they are incapable of providing any insight into the dislocation-generation mechanism. Furthermore, since the assumption of randomly spaced dislocations has been made, these results do not include the effects of special multidislocation structures (e.g., dislocation cells) which are known to be important. Computer simulation is required to include such effects.

ACKNOWLEDGMENTS

The authors gratefully acknowledge useful discussions with J. Dienes, D. Holm, P. Lomdahl, and H. Weertman. D. J. S. also acknowledges the support of the U. S. Department of Energy, Grant No. DE-FG02-88ER45367.

[1] J. P. Hirth and J. Lothe, *Theory of Dislocations* (McGraw-Hill, New York, 1982), Chap. 3.
[2] D. J. Bacon, D. M. Barnett, and R. O. Scattergood, Prog. Mater. Sci. **23**, 51 (1979).
[3] J. Weertman and J. R. Weertman, *Dislocations in Solids*, edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1980), Vol. 3, p. 1.
[4] J. Lepinoux and L. P. Kubin, Scr. Metall. **21**, 833 (1987).
[5] D. J. Srolovitz, P. S. Lomdahl, and A. Gulluoglu (unpublished).
[6] R. Eykholt and D. J. Srolovitz, J. Appl. Phys. **65**, 4204 (1989).
[7] J. D. Eshelby, Proc. Phys. Soc. London Sect. A **62**, 307 (1949).
[8] G. Liebfried and H. D. Dietze, Z. Phys. **126**, 790 (1949).
[9] J. Weertman, *Response of Metals to High-Velocity Deformation*, edited by P. G. Shewmon and V. F. Zackay (Interscience, New York, 1961), p. 205.
[10] J. P. Hirth and J. Lothe, *Theory of Dislocations* (McGraw-Hill, New York, 1982), Chap. 7.
[11] M. Peach and J. S. Koehler, Phys. Rev. **80**, 436 (1950).
[12] P. Minnhagen, Rev. Mod. Phys. **59**, 1001 (1987).