Rules for Forest Interactions between Dislocations

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The dynamical interactions of dislocations existing on intersecting glide planes have been investigated using numerical simulations based on isotropic linear elastic theory. It is found that such dislocations either repel, attract and form growing junctions, or attract and form bound crossed states. Which of these occurs can be predicted from a surprisingly simple analysis of the initial configurations. The outcome is determined primarily by the angles which the dislocations initially make with the glide-plane intersection edge, and is largely independent of the initial distance between the dislocations, their initial curvature, or ambient applied stresses. The results provide a rule for dealing with forest interactions within the context of large multiple-dislocation computations.

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Stress relaxation and plastic flow in crystals occur primarily via the motion of dislocation lines, which generate atomic slippage of the crystal at the surfaces traversed by the moving dislocations. Many phenomena such as fracture, patterning and work hardening in metals, and stress relaxation in semiconductor devices reflect the dynamical behavior of dislocations on the mesoscopic scale, and interest in modeling such behavior is growing rapidly.

The mesoscale approach (with suitable atomistic input) is well suited for exploring such problems as work hardening, where a large tangle of dislocations interacts in a complicated three-dimensional manner, while at the same time the typical spacing between dislocations is much larger than the core size. The detailed exploration of such problems requires numerical simulations, and there is intense current activity aimed at developing programs which incorporate the manifold mechanisms that govern dislocation behavior and interactions [1–8]. Our particular entrant in this field is the PARANOID code [9], a fully parallelized and highly adaptive program, designed for large calculations but also capable of resolving the behavior of individual dislocations down to nanometer scales. This latter feature permits us to examine certain key issues which must be resolved before large mesoscale simulations can be considered practical.

Dislocation-tangle simulations tend to be numerically intensive in any case. Greatly exacerbating this negative aspect, however, is the necessity of dealing with so-called *forest interactions.* By this is meant the crossing of dislocation lines moving on intersecting glide planes and often having different Burgers vectors. Such events occur only occasionally as the tangle evolves, but are of the highest importance because they lead to reconnections, the formation of jogs, junctions, and locks, and other phenomena that drastically alter the tangle dynamics. Because of the tensor nature of the interaction fields and the nonlinear character of the line dynamics, a typical forest interaction follows a complicated development to the final stage where the cores touch, atomistic calculations become appropriate, and reconnection, junction formation, or jog creation occurs. Our simulations can indeed follow this development down to nanometer scales, but to do so requires remeshing of the node density down to a 0.1 nm spacing and a concomitant reduction in the length of the time steps. Thus, to fully resolve all such interactions during a tangle simulation multiplies the computational cost by several orders of magnitude and is impractical for the systems of interest.

The consensus idea for dealing with this problem is to apply "rules" which let one jump directly from the initial configuration at which the lines begin to interact strongly to a final configuration (junction, jogs, etc.). This idea presupposes that there is a natural separation of time scales in the internal dynamics of a dislocation tangle. Typically, such dislocations move around with velocities determined by their curvature and by the applied stresses. Their effect on each other is minor, except perhaps in a mean-field sense. If two cores happen to approach each other to within a critical distance, however, their mutual interaction can take over and initiate an attractive instability which leads to a new configuration in a relatively short time. It is these events which one seeks to bypass computationally by the application of rules. If such a rule exists and two lines start to become unstable, a decision can be made based on their configuration and the lines placed into the desired outcome state. The subsequent behavior of these new configurations will again occur on relatively slow time scales—it can now be modeled in simplified terms, allowing for the growth and shrinkage of junctions, and the possible creation of jogs.

Although schematic versions of forest-interaction rules have been implemented recently [2,10], it has been far from clear that a physically realistic, useful set of such rules, in fact, exists. First, we shall see that even in the case of two initially straight lines, the interaction is complicated and seemingly unpredictable, the dislocations often twisting around substantially to find the final configuration that they favor. Second, there is a large parameter space of

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initial angles and separations to consider. Third, actual forest interactions are likely to involve curved lines, moving under large external stresses, and responding (in the case of bcc metals) with highly anisotropic mobilities, all factors which can affect their evolution in a major way. Finally, there are many distinct pairs of interacting slip systems, each of which may act somewhat differently. Indeed, it seems at first sight that the enumeration of rules becomes impossibly complicated as soon as one tries to implement it in a physically well-founded way.

In order to address this issue, we have performed a variety of forest-interaction calculations in which we follow the interactions down to the point where the cores touch. Our method of simulating dislocation dynamics has been described in Ref. [8]. Here, we first consider two straight dislocation lines lying on intersecting glide planes and having different Burgers vectors. No external stresses are applied, and the dislocations are assumed to respond with an isotropic mobility to the forces that they feel. Even for this highly simplified situation the complete parameter space of initial conditions is complicated, and we have found the following prescription to be particularly suitable for sorting things out. First, place the two lines on the edge formed by the intersecting glide planes and pick a common point P on this edge. Rotate each line about P on its own glide plane by an angle ϕ_1 and ϕ_2, respectively, and then displace the lines a distance d_1 and d_2, respectively, in the direction perpendicular to the rotated line [Fig. 1(a)]. The result for any particular forest interaction described in this way by a particular initial condition, ϕ_1, ϕ_2, d_1, d_2, was found to be sensitive to ϕ_1 and ϕ_2, but not to d_1 and d_2. The latter could generally be varied from ± 20 to ± 400 nm without much effect, and this dependence will be suppressed during the following discussion.

For certain ranges of ϕ_1, ϕ_2, the two lines shown in Fig. 1(a) have a repulsive interaction. In the absence of external stresses or line-curvature effects, the dislocations then drift apart in an uninteresting manner. When ϕ_1, ϕ_2 are such that the interaction is attractive, however, the lines come together to form a bound state. Often, this bound state takes the expected form of a junction [Figs. 2(a) and 2(b)] in which the two dislocations combine and zip up until the process is halted by extraneous factors such as pinning. In more cases than not, however, our calculations indicate that the dislocations end up in a *crossed* state [Figs. 2(c) and 2(d)], which is bound but which does not zip up to form a junction. The existence of these stable states has little to do with core interactions, the crosses remaining bound even if the cores of dislocations are moved freely through each other. Since discussions of forest interactions in the literature have focused exclusively on junctions as the primary actors in dislocation-tangle dynamics, the prevalence of these crosses seems very surprising, and their possible significance deserves further study.

We now consider the question of predicting the outcome of a forest interaction. Figure 3(a) shows the results of fully resolved runs for a particular pair of bcc slip systems. Each point in the figure corresponds to a complete run involving two initially straight lines oriented at angles ϕ_1, ϕ_2 with respect to the glide-plane edge as illustrated

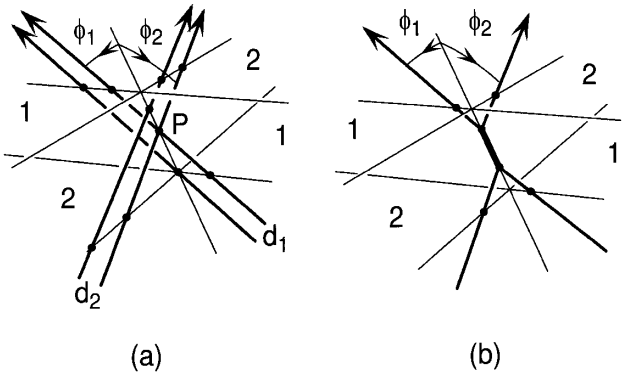

FIG. 1. Geometric conventions: (a) Each dislocation has an initial angle ϕ with respect to the glide-plane edge, taken in the direction given by the cross product of normal with edge vector. The initial angles ϕ_1, ϕ_2 relate to the calculated final state as shown by the symbols in Fig. 3. (b) Hypothetical junction construction used with Eq. (1) to *predict* the final state. Although dislocations may twist to new orientations during junction formation, analysis of this configuration successfully separates junction-forming and nonforming initial conditions via the contours shown in Fig. 3.

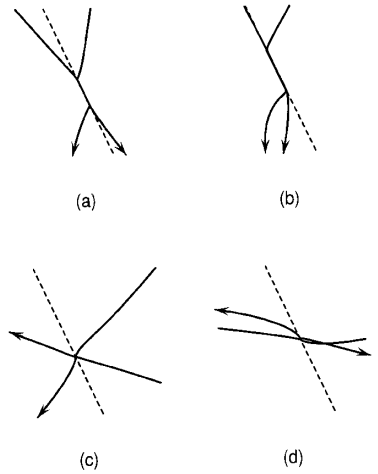

FIG. 2. Many pairs of attracting dislocations, such as (a) in this figure, evolve to resemble textbook pictures of straight-armed junctions. Other pairs link in a simple cross shape, but do not zip together to form a junction [Fig. 1(c)]. In other circumstances, both zipping and nonzipping cases show a substantial amount of local twisting [e.g., (b) and (d), which have been magnified by a factor of 10]. These simulations used the slip system pair of Fig. 3(a), with isotropic mobility and no external stress. Initial configurations were as shown in Fig. 1(a), with angles $\phi_1 = -150°$, $\phi_2 = -150°$; $\phi_1 = 180°$, $\phi_2 = -120°$; $\phi_1 = 90°$, $\phi_2 = -120°$; $\phi_1 = -90°$, $\phi_2 = -120°$.

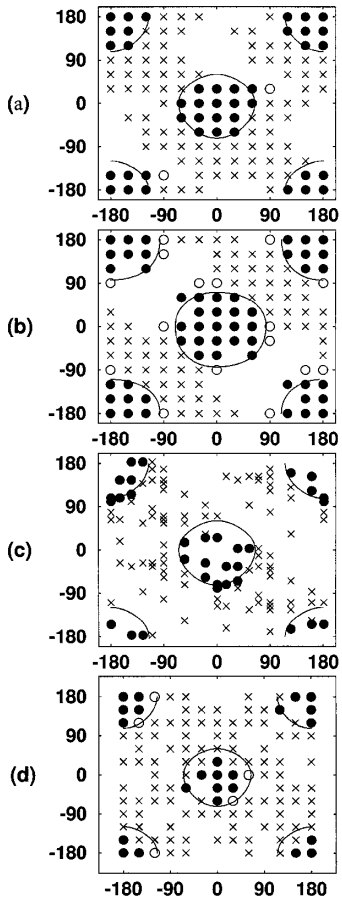

FIG. 3. (a) and (b) show the behavior of two initially straight dislocations under zero external stress. Filled circles represent the formation of well-defined junctions, crosses indicate bound crossed states, and hollow circles show borderline cases which zipped up less than a nanometer during the simulation period. Empty spaces indicate repulsive dislocations in (a) and (b). (a) shows the bcc pair $(0\bar{1}1)\frac{1}{2}[1\bar{1}\bar{1}]$ and $(\bar{1}01)\frac{1}{2}[111]$, while (b) shows the bcc pair $(110)\frac{1}{2}[1\bar{1}\bar{1}]$ and $(\bar{1}01)\frac{1}{2}[111]$. (c) involves the same pair of slip systems as (a), but here one of the dislocations starts out as a circular loop of radius 30–100 nm. (d) shows results for the same slip systems as (a), but now the calculations are carried out with the addition of a large (690 MPa) uniaxial stress.

in Fig. 1(a). We observe that while all attractive interactions lead to bound states, true junction formation occurs only in compact, localized regions of ϕ_1, ϕ_2 parameter space. The interesting question is whether this outcome can be predicted without doing such detailed calculations.

Figure 1(b) illustrates the textbook way of viewing a junction [11]. To analyze whether such an idealized junction is energetically favored (i.e., wants to grow), one considers the energy change

$$f = -\delta(E_1 + E_2 + E_3)/\delta x \qquad (1)$$

due to a virtual displacement δx of one of the junction ends along the glide-plane edge. In the usual simple application of this argument to an isotropic system, one uses the energy per unit length

$$E = \frac{\mu b^2}{4\pi(1-\nu)}(1 - \nu\cos^2\beta)\ln(R/a) \qquad (2)$$

for each arm to determine its contribution to the energy balance. Here, μ is the shear modulus, ν is Poisson's ration, $\vec{b}$ is the particular Burgers vector $\vec{b}_1$, $\vec{b}_2$, or $\vec{b}_1 + \vec{b}_2$ appropriate to the arm, β is the angle between this Burgers vector and the arm direction, and $\ln(R/a)$ is the usual phenomenological core cutoff term. As noted by Herring [12], $\delta E/\delta x$ involves not only line tension contributions from changes in the arm lengths, but also "torque" terms arising from changes in the directions of arms one and two. The interaction energy between the various branches is ignored, and indeed one might guess that such interactions will significantly alter the idealized shape usually shown in the textbooks.

At first sight, this simple model seems to have little relation to a junction formed on the fly where, as shown in Figs. 2(b) and 2(d), the lines will often twist around quite dramatically to make (or avoid making) a junction. In particular, the final orientations of the arms near the junction are generally quite different from their starting orientations. Remarkably, however, we find that Eqs. (1) and (2) applied to the idealized junction shown in Fig. 1(b) are sufficient to predict the outcome of a forest interaction, provided that the *initial* orientations ϕ_1, ϕ_2 of the interacting lines are used to specify the orientations of the "trial junction" arms, as indicated in Fig. 1. The contours drawn in Fig. 3(a) show the regions of ϕ_1, ϕ_2 space where the idealized trial junction is energetically favored, and indeed our detailed calculations show that all of the initial conditions lying within the junction contour lead to the eventual formation and growth of a stable junction. For other values of ϕ_1, ϕ_2, attractive interactions lead to the formation of crossed states.

These results appear to be quite general. Figure 3(b) shows a study done for a different pair of bcc slip systems. Again, the analysis based on Eqs. (1) and (2) works remarkably well. We note that although Figs. 3(a) and 3(b) are similar, they differ significantly in detail, indicating that the analysis yields important quantitative information. Results similar to Figs. 3(a) and 3(b) are obtained for other interacting bcc slip systems, as well as for fcc systems.

Predictions based on the analysis we have described are found to be remarkably robust. It has already been pointed out that the observed (computed) final configurations are quite insensitive to the signs and magnitudes of d_1 and d_2. However, in a real system of interacting dislocations, forest interactions will usually involve a host of other complications. Typically, the dislocations may experience large external stresses, they may be highly curved when they encounter each other, and their response to the forces they experience may be highly anisotropic [13]. Each of these factors has a major influence on the

dislocation motion. Nevertheless, we find that they have relatively little effect on the final outcome of the interaction. Figures 3(c) and 3(d) show the effects of line curvature and stress for the slip systems shown in Fig. 3(a). Even under situations where the dynamical behavior is disturbed greatly by these complications, or where it becomes rather difficult [14] to define the asymptotic initial conditions ϕ_1, ϕ_2, the predictive power of Eqs. (1) and (2) is still quite remarkable. Such deviations from Fig. 3(a) as can be observed in Figs. 3(c) and 3(d) seem largely to arise from the fact that when the initial curvatures or the applied stresses are large, the motion of the dislocations far away from the interacting region speeds up greatly. The asymptotic conditions then change significantly during the time it takes the junction or crossed state to form, and the separation of time scales discussed earlier begins to break down [15].

We conclude that the application of Eqs. (1) and (2) to the initial configuration largely suffices to predict whether any particular forest interaction will lead to junction or cross formation. This implies that it is the asymptotic directions that the junction arms would have in the absence of interactions, and not the orientations which they actually assume very near the junction, which determine junction stability. The results are surprisingly robust, depending only marginally on initial line separation, line curvatures, ambient stresses, and mobility anisotropy. The analysis we have outlined is trivial to implement computationally: When two dislocation lines approach to where their mutual interaction becomes significant, a subroutine is accessed which constructs the idealized junction and applies Eqs. (1) and (2) to see whether it wants to grow or shrink. If the idealized junction is stable (growing), the program reconstructs the dislocations into a junction configuration. If not, it generates a crossed configuration. Thus the subroutine plays the role of the desired rule and is currently being implemented as a part of our large-scale dislocation-tangle simulations.

A second important outcome of the work presented here is the observation that the majority of attractive interactions lead not to junctions but to crossed states. In addition, we have found that, if repulsively interacting dislocations are forced together by an applied stress, crossed states, not junctions, are formed [Fig. 3(d)]. Some, but not all, of both the crosses and the junctions persisted for significant periods of time under the 690 MPa external stress used for the runs in Fig. 3(d), an observation which indicates that the topological constraints produced by crosses may be of comparable strength to those of many junctions. Although further calculations, perhaps on the atomistic level, will be required to explore this issue, it appears that the crossed states configurations may also represent important obstacles to motion in the dynamics of interacting dislocations.

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[11] Because reversing both the Burgers vector and the direction of a dislocation leaves things unchanged, there is an ambiguity in the definition of ϕ_1, ϕ_2. We define line and Burgers vector directions such that $|\vec{b}_1 + \vec{b}_2|^2 \leq |\vec{b}_1|^2 + |\vec{b}_2|^2$, so that junctions consist of parallel lines.
[12] C. Herring, in *The Physics of Powder Metallurgy*, edited by W. E. Kingston (McGraw-Hill, New York, 1949).
[13] In bcc metals it is not unusual for the mobility of edgelike segments to be 2 orders of magnitude greater than the mobility of screwlike segments.
[14] For forest interactions where the dislocations are significantly curved when they begin to interact strongly, the "initial angles" ϕ_1, ϕ_2 are defined by drawing tangents through the dislocation curves at the points of closest approach.
[15] It is possible that the fit in Fig. 3(d) could be improved further by including external stress effects in the energy-balance arguments of Eqs. (1) and (2). We note, however, that a stress of 140 MPa yields results which are virtually indistinguishable from the zero-stress results shown in Fig. 3(a).