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Mobility laws in dislocation dynamics simulations

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Abstract

Prediction of the plastic deformation behavior of single crystals based on the collective dynamics of dislocations has been a challenge for computational materials science for a number of years. The difficulty lies in the inability of existing dislocation dynamics (DD) codes to handle a sufficiently large number of dislocation lines, to establish a statistically representative model of crystal plasticity. A new massively parallel DD code is developed that is capable of modeling million-dislocation systems by employing thousands of processors. We discuss an important ingredient of this code — the mobility laws dictating the behavior of individual dislocations. They are materials input for DD simulations and are constructed based on the understanding of dislocation motion at the atomistic level.

Keywords: Crystal plasticity; Dislocation dynamics; Mobility

1. Introduction

Under a wide range of stress and temperature conditions, the plastic deformation of a crystal is produced by the motion of dislocation lines through the lattice [1]. This *qualitative* picture has been well known for several decades, since the theoretical postulate of the dislocation model and the experimental observation of dislocation microstructures in deformed materials. However, *quantitative* prediction of the plastic strength of a single crystal based on dislocation dynamics (DD) remains a grand challenge to date. The bottleneck seems to be a technical one. To construct a representative model of crystal plasticity, the dynamics of a *large enough* number of dislocations needs to be followed for a *long enough* time. The length and time scales it requires remains out of reach of existing simulation codes. A new massively parallel DD code is developed that significantly extends the capability of DD simulations. A general description of this code, DD3d, was given in [2]. In the present paper, we focus on a specific methodological issue: how to construct mobility laws to describe the behavior of individual dislocations in a DD simulation.

In DD3d dislocations are represented as a set of "nodes" connected with each other by straight line segments, as shown in Fig. 1. If a node is connected with n other nodes, it is called an n-node. Most of the 2-nodes merely serve as discretization points of the dislocation line, and are hence called *discretization nodes*, such as nodes 1–3 in Fig. 1. On the other hand, multi-arm nodes, such as node 0, are "physical"-nodes, as it represents a physical location where several dislocations meet together. Occasionally a 2-node can also be a physical node, such as the cusp left on a dislocation after cross slip.

A DD simulation is nothing but the numerical integration of the nodal equation of motion, which is usually assumed to be over-damped and takes the following form:

$$\vec{v}_i \equiv \frac{\mathrm{d}\vec{r}_i}{\mathrm{d}t} = M(\vec{f}_i) \tag{1}$$

$$\vec{f}_i \equiv \frac{\mathrm{d}E_{\mathrm{el}}(\{\vec{r}_i\})}{\mathrm{d}\vec{r}_i} \tag{2}$$

where $\vec{r}_i$, $\vec{v}_i$, $\vec{f}_i$ are the position, velocity and force on node i, respectively. E_{el} is the total elastic energy of the dislocation network. The computation of nodal forces from Eq. (2) can be carried out based on analytic formula developed within linear elasticity theory [1–3]. This is the *generic* part of DD3d, meaning that it requires only a minimal amount of material specific input such as the elastic constants. Hence the same machinery can be used to describe different materials without any significant change.

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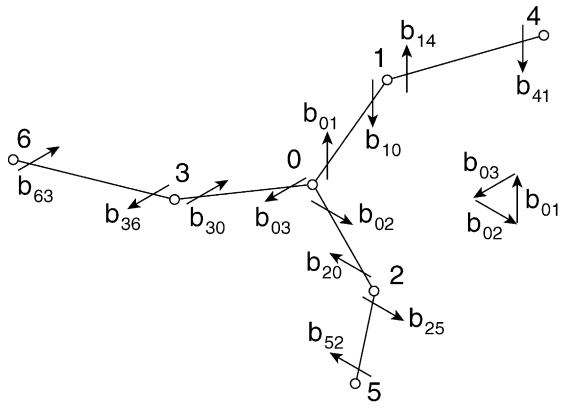

Fig. 1. Dislocation network represented as a set of "nodes" interconnected by straight segments. The Burgers vectors are defined on every arm with line direction pointing away from the node. For example, $\vec{b}_{01}$ is the Burgers vector of the arm going from node 0 to node 1, and $\vec{b}_{10}$ is the Burgers vector of the same arm going in the reverse direction. Consequently there exist sum rules for every arm, e.g. $\vec{b}_{01} + \vec{b}_{10} = 0$, and for every node, e.g. $\vec{b}_{01} + \vec{b}_{02} + \vec{b}_{03} = 0$.

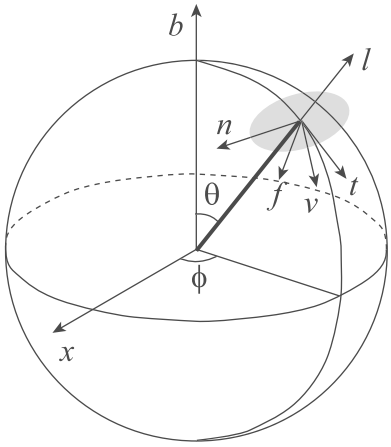

Fig. 2. Geometry of vectors in mobility function $\vec{v} = M(\vec{f}, \theta, \phi)$. $\vec{b}$ and $\vec{l}$ are dislocation Burgers vector and line direction, respectively. The unit vector $\vec{n}$ is the glide plane normal, i.e. $\vec{n} \| \vec{l} \times \vec{b}$, and unit vector $\vec{t}$ is parallel to $\vec{l} \times \vec{n}$. Both dislocation velocity $\vec{v}$ and driving force $\vec{f}$ are 2-dimensional vectors in the tangent (shaded) plane spanned by $\vec{n}$ and $\vec{t}$ (see text).

On the other hand, the computation of nodal velocities in response to the driving forces, as in Eq. (1), is strongly *material specific*. This is because how dislocations move is largely controlled by the atomistic structures and energetics of the dislocation core, which can vary significantly from one dislocation (or material) to another. Such information is beyond the realm of linear elasticity theory and can only be obtained from more detailed, atomistic-level simulations. For example, a molecular dynamics (MD) simulation can compute the velocity of a specific dislocation under a given temperature and stress condition [4]. However to make such data accessible to DD simulations, they need to be assembled into a "constitutive law", which describes the dislocation velocity as a function of temperature, force, and dislocation characters.

2. Mobility of discretization nodes

For simplicity we will neglect the temperature dependence, i.e. we will consider DD simulations at a fixed temperature. We will also limit our discussion to the mobility of discretization nodes. Because these nodes are sampling points of a presumably smooth dislocation line, it suffices to consider the velocity function of differential dislocation segments, $\vec{v} = M(\vec{f}, \vec{l}, \vec{b})$, where $\vec{f}$ is the force per unit length, $\vec{l}$ the line direction and $\vec{b}$ the Burgers vector, as in Fig. 2. Equivalently we can write the velocity function as $\vec{v} = M(\vec{f}, \theta, \phi)$, where θ and ϕ describe the orientation of $\vec{l}$ with respect to $\vec{b}$. Because motion of a line along itself is unphysical, we restrict $\vec{v}$ and $\vec{f}$ to the 2-dimensional space perpendicular to $\vec{l}$.

To use this mobility law in a node-based code such as DD3d, we need to translate nodal information into segment properties $\vec{f}$ and $\vec{l}$. Consider for example a discretization node i with two neighbors, 0 and 1. We can approximate the local dislocation line direction near node i to be $\vec{l} = (\vec{r}_1 - \vec{r}_0)/|\vec{r}_1 - \vec{r}_0|$ and the force per unit length to be $\vec{f} = \vec{f}_i/L$, where

$$L = \tfrac{1}{2}|\vec{r}_1 - \vec{r}_0| \tag{3}$$

3. A simple FCC model

The simplest mobility law is perhaps the one that describes the generic dislocation behavior in face-centered-cubic (FCC) metals (e.g. Cu, Al) in low temperatures. Let us call it FCC0. Here we focus on ordinary dislocations with 1/2 $[1\,\bar{1}\,0]$ type Burgers vectors. The core of this dislocation splits planarly into two partials on (1 1 1) planes, bounding a stacking fault area. As a result, dislocation motion is entirely confined within the dissociation plane, except for cross slip events which will be discussed later. Ignoring cross slip, the glide plane normal vector $\vec{n}$ remains the same as specified in the initial condition. It should be taken into account as an extra input for the mobility law function, i.e., $\vec{v} = M(\vec{f}, \vec{l}, \vec{b}, \vec{n})$..

For simplicity, we can assume that dislocation velocity is isotropic within the glide plane. We may also assume that dislocation velocity is linear to the driving force. This is a reasonable approximation because the Peierls stress (the critical stress below which dislocation does not move at 0 K) in FCC metals is very low. Thus, we arrive at a mobility law described by a single parameter M,

$$\vec{v} = M \cdot \vec{f} - M \cdot (\vec{f} \cdot \vec{n}) \cdot \vec{n} \tag{4}$$

The second term ensures that velocity $\vec{v}$ remain orthogonal to glide plane normal $\vec{n}$. The mobility coefficient M can be determined from a molecular dynamics simulation at a constant stress. In general M can depend on temperature T

and function $M(T)$ can be constructed from MD simulations at different temperatures [4].

More complex effects can be added to this simple mobility law, to describe dislocation behavior more accurately. For example, M can be angular dependent, such as, $M(\theta) = M_s \cos^2\theta + M_e \sin^2\theta$, where M_s and M_e are two parameters describing the mobility of screw and edge dislocations, respectively. More generally, dislocation velocity is a non-linear function of driving force, if non-relativistic effects are of interest when dislocation velocity approaches sound velocity, such as under shock conditions. However, the most important improvement to the above mobility law should be the incorporation of cross slip. For a dislocation with Burgers vector $1/2\,[1\,\bar{1}\,0]$, its glide plane could be either $(1\,1\,1)$ or $(1\,1\,\bar{1})$. When the local line direction is parallel to the Burgers vector (screw orientation), there is a finite probability for the node to flip its glide plane normal from one to the other, i.e., to cross slip. The cross slip probability P_x is a function of local driving force (per unit length) $\vec{f}$. For the simulation result to be independent from the choice of spatial and temporal discretization, P_x should be proportional to the segment length L the node represents [Eq. (3)] as well as waiting time Δt, which can be the simulation time step. Thus P_x can be written as

$$P_x = J_x(\vec{f}) \cdot S(\theta) \cdot L \cdot \Delta t \tag{5}$$

where function $S(\theta)$ equals 1 when $\theta = 0$ and quickly goes to 0 as $|\theta|$ increases. The cross slip rate function $J_x(\vec{f})$ can be constructed based on atomistic simulation results.

4. A simple BCC model

While the above mobility law makes sense for FCC metals, it would have difficulty if applied to body-centered-cubic (BCC) metals. Dislocations in BCC metals do not dissociate into partials as they do in FCC metals. The cores of screw dislocations are especially compact and consequently can move on several planes with equal tendency. Therefore, introducing a glide plane for screw dislocations would be rather artificial. If the above FCC mobility law were applied to BCC metals, a very high cross slip probability would have to be used. As a result a long screw dislocation would very quickly be divided into short segments moving in different planes. The result would depend on the discretization length and be rather unphysical. The problem is made more serious by the low mobility of screw dislocations compared with non-screw dislocations, which leads to a high percentage of screw segments in the dislocation population. Therefore, it is very important to have a good account for screw dislocations in BCC mobility laws.

In this section we derive a simple mobility law, BCC0, which captures the generic behavior of dislocations in BCC metals. To make progress, let us start from an opposite point of view to that of FCC0 and assume that screw dislocations can move in all directions with isotropic mobility. This means that when $\theta = 0$,

$$\vec{v} = M_s \cdot \vec{f} \tag{6}$$

However, the mobility of non-screw dislocations should still be highly anisotropic. When $\vec{l}$ is not parallel to $\vec{b}$, a glide plane can be defined with normal vector $\vec{n} = (\vec{l} \times \vec{b})/|\vec{l} \times \vec{b}|$. The glide motion within the plane will be much faster than the climb motion out of the plane. To construct an analytic function that describes $\vec{v}(\vec{f}, \theta, \phi)$ for all line directions, the typical non-screw behavior should transform smoothly to the screw behavior, as θ goes to 0. Therefore, climb motion for non-screw dislocations, which was completely suppressed in FCC0, should be allowed here. The difference between glide and climb mobility of non-screw dislocations, which can be quite large for large θ, should conveniently vanish as θ goes to 0, for which the glide plane cannot be defined in the first place.

One way to construct such a mobility law is to consider the physics of dislocations in near screw orientations ($\theta \approx 0$) and extrapolate the expression to all orientations. Atomistic simulations have found that a screw dislocation in BCC metals lies along an energetically favorable direction and experiences very high lattice resistance [5]. The motion of screw dislocation is typically carried out by thermal-assisted kink-pair nucleation. Once the kinks are nucleated, they quickly move away for long distances before annihilating with other kinks. As a result, the screw dislocation moves forward by one lattice distance h.

If the dislocation line direction $\vec{l}$ is slightly tilted away from the Burgers vector $\vec{b}$, the dislocation will still assume screw character along most of its length, and account for the deviation by making kinks with atomic height h. The tilt angle θ is related to the average separation between kinks D through $\tan\theta = h/D$. Because the typical width of this kink is around $5h$, dislocations can be considered as a combination of screw segments and kinks as long as $\theta < \arctan(1/5) \approx 10^\circ$. In the following we will construct mobility law functions using the screw-and-kink model for dislocations within the vicinity of screw orientations. As an approximation, we will then extrapolate the resulting function to describe mobility of all dislocations.

Let us first consider the glide motion of dislocations vicinal to screw orientations, and let $f_t = \vec{f} \cdot \vec{t}$ be the glide component of the driving force. The "geometrically necessary" kinks that accommodate the dislocation's non-screw character can give dominant contribution to dislocation velocity at large θ. Let the kink velocity be $v_k = M_k f_t$, with M_k being the kink mobility. The dislocation velocity would then be $v \approx v_k \sin\theta = M_k f_t \sin\theta$. On the other hand, when θ is very small, $v \approx M_s f_t$. A smooth function that connects these two behaviors is

$$v = (M_s^2 + M_k^2 \sin^2\theta)^{1/2} f_t \equiv M_t(\theta) f_t \tag{7}$$

We now consider the climb motion of dislocations vicinal to screw orientations and let $f_n = \vec{f} \cdot \vec{n}$ be the climb component of the driving force. The screw segments cannot tell the difference from the above situation because their mobility is isotropic. However, in this case, the kinks will have to climb, which is much more difficult than gliding. The entire dislocation has to move together, so that the slow moving kinks (in this orientation they are usually called jogs) will exert a drag on the screw segments. Let M_j be the climb mobility of jogs. A similar argument as the above would suggest the following equation:

$$v = (M_s^{-2} + M_j^{-2} \sin^2\theta)^{-1/2} f_n \equiv M_n(\theta) f_n \tag{8}$$

We notice that when $\theta \to 0$, Eqs. (7) and (8) both converge to Eq. (6), as they should. Combining these two equations, the mobility function can be written explicitly as

$$\vec{v} = [M_t(\theta)\vec{t} \otimes \vec{t} + M_n(\theta)\vec{n} \otimes \vec{n}]\vec{f} = M_t(\theta)\vec{f} - [M_t(\theta) - M_n(\theta)](\vec{n} \cdot \vec{f})\vec{n} \tag{9}$$

Notice that $\vec{b} \times \vec{l} = \vec{n} \sin\theta$, we have

$$\vec{v} = M_t(\theta)\vec{f} - \frac{M_t(\theta) + M_n(\theta)}{\sin^2\theta}[(\vec{b} \times \vec{l}) \cdot \vec{f}](\vec{b} \times \vec{l}) \equiv M_t(\theta)\vec{f} - g(\theta)[(\vec{b} \times \vec{l}) \cdot \vec{f}](\vec{b} \times \vec{l}) \tag{10}$$

One can show that function $g(\theta)$ is a well-defined and continuous function for all θ and $g(0) = (1/2)M_s[(M_k/M_s)^2 + (M_s/M_j)^2]^{1/2}$.

Eq. (10) specifies the mobility of a generally orientated dislocation segment in BCC metals by three parameters, M_s, M_k and M_j. Alternatively, we can redefine M_k and M_j by new variables such as $M_g \equiv M_t(\theta = 90^\circ)$ and $M_c \equiv M_n(\theta = 90^\circ)$,

$$M_k = (M_g^2 - M_s^2)^{1/2}$$

$$M_j = (M_c^{-2} - M_s^{-2})^{-1/2}$$

and define the general mobility function in terms of M_s (screw mobility), M_g (edge dislocation glide mobility) and M_c (edge dislocation climb mobility). The physical values for these three parameters can be obtained from atomistic simulations. Typically $M_g \gg M_s \gg M_c$.

The mobility law as defined in Eq. (10) is numerically well-behaved and provides a simple model of dislocations in BCC metals. The parameters in this model all have physical meaning and can be determined from atomistic simulations or from experimental measurements. For example, both the kink mobility M_k and glide mobility of edge dislocation M_g have been computed by molecular dynamics simulations in BCC molybdenum [4]. At $T = 300$ K, they are found to be $M_k = 2.22 \times 10^4$ and $M_g = 5.56 \times 10^3$ Pa^{-1} s^{-1}. This mobility law can also be made more complex to describe the physics of dislocation motion more realistically. A major improvement would be to replace the completely isotropic mobility of screw dislocations. Screw dislocations assume isotropic only at relatively high temperatures and this phenomena is called *pencil glide*. At lower temperatures, the motion of screw dislocations is tilted certain crystallographic [such as $(1\,\bar{1}\,0)$] planes. The velocity is not necessarily parallel to the force direction. The mobility function can be modified to take the anisotropic effect into account. However, we emphasize that even in this case, the behavior is still very different from the FCC0 model — the velocity is solely determined by the driving force $\vec{f}$ and there exists no internal variable such as the glide plane normal $\vec{n}$ as in FCC0.

A more realistic mobility model would have non-linear force–velocity relationship. In BCC metals this becomes more important because of the higher lattice resistance for screw dislocations. The velocity would show non-linear behavior as the force becomes comparable to the lattice resistance. Eq. (10) also has axial symmetry along the Burgers vector axis. In reality this symmetry can be broken, for example, when certain crystallographic directions other than the screw orientation are also energetically favored. For example, atomistic simulations have found that the mixed-71° dislocation, for which $\vec{b} = [1\,1\,1]$ and $\vec{l} = [1\,1\,\bar{1}]$ also has a distinctive and favored core structure [3]. Line directions in its vicinity may also be modeled as a combination of straight 71°-segments and kinks, similar to the case of dislocations vicinal to screw orientation. The mobility function taking this into account would lose the axial symmetry but would always retain certain crystallographic symmetry of the lattice.

5. Summary

In this paper, we describe how atomistic information on the dislocation core can be used to construct mobility laws, which serve as inputs for the equation of motion in dislocation dynamics simulations. This is the approach we take to develop the new massively parallel DD code DD3d. Although the reason that DD3d can efficiently utilize thousands of processors in parallel is not due to the mobility laws per se, the successful implementation of the parallel computation does benefit significantly from a clear separation of the material specific component — the mobility law, from the remaining generic components of the DD model.

We have described two simple models as examples on how mobility-law functions can be constructed to reflect the essential physics of dislocation motion. For FCC metals where cross slip can be ignored, the confinement of dislocation motion to the glide plane is taken into account simply by orthogonalizing dislocation velocity to the plane normal. For BCC metals, because non-screw dislocations are confined to move in the glide plane while screw dislocations are not, a more complicated functional form is required to capture this transition smoothly. The simplest model satisfying this requirement can be described by three parameters, which can be determined by either molecular dynamics simulations or experimental measurements.

It is interesting to look at the mobility law as a *constitutive equation* of a single dislocation. It is provided by atomistic simulations, which takes the interaction between individual atoms as input and studies the collective behavior of many atoms. The task of DD simulation is to take this as input, study the collective behavior of many dislocations, and eventually produce a *constitutive equation* for the plastic strength of a single crystal. It is not difficult to imagine a continuum model that takes the single crystal *constitutive equation* as input, studies the collective behavior of many crystal grains, and eventually produces a *constitutive equation* for a polycrystal. A hierarchical pattern emerges here, where a *constitutive equation* repeatedly serves as the link between a lower-scale model and a higher-scale one. This is one of the several approaches for the intrinsically hard, multi-scale problems and appears very promising in the pursuit towards understanding crystal plasticity.

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