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ABSTRACT

The aim of this contribution is to present the current state of our research in the field of numerical simulation of dislocation motion in crystalline materials. The simulation is based on recent theory treating dislocation curves and dipolar loops interacting by means of forces of elastic nature and hindered by the lattice friction. The motion and interaction of a single parametrically described dislocation curve and one or more dipolar loops placed in 3D space is considered. The complexity of the stress fields of dipolar loops as well as of the dislocation curve necessitates application of advanced numerical algorithms to successfully solve the problem. The present numerical algorithm is based on analytical formulae for stress tensor of interaction between dislocation curve and dipolar loop, analytical interaction formulae for dipolar-to-dipolar loop interaction, parametric description of the dislocation curve (i.e. 1D description of a fully 3D problem), and the flowing finite volume method. It is showing up, that despite of using analytical formulae in the numerical algorithm, it is necessary to introduce distance thresholds for evaluation of these formulae.

1. Numerical Model

In our model of dislocation dynamics, discrete solution of the dislocation curve is represented by a moving polygon given, at any time \( t \), by plane points \( \vec{X}_i, i = 0, \ldots, M \). The values \( \vec{X}_0 \) and \( \vec{X}_M \) of the end points are prescribed in case of fixed ends of the curve, i.e. the values do not depend on time. The segments \( [\vec{X}_{i-1}, \vec{X}_i] \) are called flowing finite volumes. The evolution equation of the dislocation curve has the form of intrinsic diffusion equation [3], [1], [2], [5]. By integrating in dual volumes and using some other straightforward steps described in [8] we get a system of ordinary differential equations for the points of the polygon:

\[
B \frac{d\vec{X}_i}{dt} = \varepsilon \left( \frac{2}{d_i + d_{i+1}} \left( \frac{\vec{X}_{i+1} - \vec{X}_i}{d_{i+1}} - \frac{\vec{X}_i - \vec{X}_{i-1}}{d_i} \right) + \frac{2}{d_i + d_{i+1}} F_i \frac{\vec{F}_i \vec{X}_{i+1} - \vec{F}_i \vec{X}_{i-1}}{2} \right), \quad i = 1, \ldots, M - 1.
\]
In the above ODE system, $d_i$ denote distances between neighbouring nodes of the dislocation curve’s discretization. Obviously, we have to complete the ODE system by including differentials $\frac{dX_0}{dt}$ and $\frac{dX_M}{dt}$. The exact form of these differentials depends on the particular model we use.

The governing equations for the motion of dipolar loops, that are allowed to move only along the x-axis, consist of another system of ODE:

$$\frac{dx^{(j)}(t)}{dt} = \frac{1}{BP} F_{x,total}^{(j)}(X_0(t), \ldots, X_M(t), x^{(0)}(t), \ldots, x^{(N)}(t)), \quad j = 1, \ldots, N,$$  \hspace{1cm} (2)

where $x^{(j)}(t)$ denotes the x-axis position of the j-th dipolar loop, and $F_{x,total}^{(j)}$ (depending on positions of the dislocation curve and all the other dipolar loops) denotes the total forces acting on the j-th dipolar loop.

The complete discrete problem consists of (1) and (2) with accompanying initial and boundary conditions. The initial conditions simply describe positions and shapes of the dislocation curve and dipolar loops at the beginning of the computation. The boundary conditions differ depending on the particular model (both mathematical and numerical) we solve. The terms $F_i$ in Eqn (1) and $F_{x,total}^{(j)}$ in Eqn (2) are very complex and include stress fields of dipolar loops as well as the interactions among the dipolar loops, which both are also very complex.

The interaction between two dipolar loops in stable configurations is described by analytical formulae which were presented in [6]. The analytical formula for the stress field generated by a single dipolar loop of type $V_1$, $V_2$, $I_1$, or $I_2$ is based on the formula presented by Kroupa in [4]. Due to some special arrangements of our model it reads:

$$\sigma_{xy}(x, y, z) = -\frac{\mu hb}{2\pi (1 - \nu)} \left\{ \frac{l - z}{\varrho_-} + \frac{l + z}{\varrho_+} \right\} \left[ \frac{x \pm y}{(x^2 + y^2)^2} \left( \pm x + y - 8 \frac{x^2 y}{x^2 + y^2} \right) + \frac{l}{\varrho_-^3} + \frac{l + z}{\varrho_+^3} \right] \left[ \pm \nu + \frac{xy}{(x^2 + y^2)^2} \left( y^2 - 3x^2 \mp 4xy \right) \right] + \frac{l}{\varrho_-^5} + \frac{l + z}{\varrho_+^5} \right\} \left[ -3x^2 y(x \pm y) \right], \hspace{1cm} (3)$$

$$\varrho_- = \sqrt{x^2 + y^2 + (l - z)^2}, \quad \varrho_+ = \sqrt{x^2 + y^2 + (l + z)^2},$$

where $\sigma_{xy}$ stands for the xy-component of the stress field tensor, $x, y, z$ is the relative position of the point we want to evaluate the stress in, $\mu$ is shear modulus, $h$ and $l$ are the half-width and half-length of a dipolar loop, $b$ is Burgers vector, and $\nu$ is Poisson’s ratio.

2. Stress Field Evaluation Threshold

Having the analytical formula for the stress field $\sigma_{xy}$ and the interaction force of a pair of dipolar loops may seem to be enough for fast computation. However, this is not true. According to the

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1Each dipolar loop is described by a letter and a subindex. Letters $V$ and $I$ stand for vacancy and interstitial dipolar loops, subindices 1 and 2 denote stable configurations as presented in [8], [7].
profiling results of disdyn\textsuperscript{2} code for a test case having single dislocation curve and 10 dipolar loops, about 93\% of CPU time was spent in computation of $\sigma_{xy}$ and about 5\% in computation of interactions among dipolar loops. The rest was spent in Runge-Kutta and other supplemental algorithms.

![Figure 1](image_url)

Figure 1. Stress field dependency on the z-axis distance from the plane of dipolar loop

With employment of a cut-off distance for $\sigma_{xy}$ computation, which was set to 50 nm\textsuperscript{3}, the profiling results were much better. CPU time spent in computation of $\sigma_{xy}$ fell down to about 60\%, while the unchanged (i.e. still not using the threshold) interaction force among dipolar loops arised to 20\%.

As was already written, the numerical scheme uses analytical formulae for evaluation of the stress field generated by a single dipolar loop and the interaction force between a pair of dipolar loops. Both of these are complex formulae which proved to be time expensive to evaluate. More precisely, they are fast to evaluate for a single set of parameters, but we need to evaluate them very often. Indeed, according to the test simulation (with 10 dipolar loops and one dislocation curve consisting of 2000 segments) running in a profiler we learned that about 93\% of the time the program is running, it is in the procedure of evaluation the stress field generated by a single dipolar loop. Another 5\% it spends inside the evaluation of the formula of the interaction between two dipolar loops.

\textsuperscript{2}The computational program developed to implement numerical simulation of dislocation dynamics

\textsuperscript{3}Where such a cut-off value comes from? We will explain later in this section
Obviously, these numbers depend on the exact setting of the test simulation; they will change with a different setting of the number of segments of the dislocation curve and the number of dipolar loops. Just for imagination, in the setting we profiled, a particular time step of Runge-Kutta method consists of 159960 evaluations of the stress field and 360 evaluations of interactions between a pair of dipolar loops. Therefore, the first motivation for improving the speed of the algorithm came from the fact we wanted to run our model with a bigger amount of dipolar loops. The second motivation was the speed itself which was not good even for a very small amount of dipolar loops.

2.1 Optimizing the stress field evaluation

There is a simple idea how to make the stress field evaluation faster. The stress field is evaluated many times during the algorithm, and many times it evaluates to a value which is near to zero. This is because of the fact that the stress field is of a short-range type and vanishes very quickly as the distance from the generating dipolar loop is growing. Thus, putting a threshold distance into the algorithm seems to be straightforward. We simply neglect the stress generated by a dipolar loop if the point, at which we want to evaluate the stress, is far enough from the dipolar loop.

However, it is not an easy task to setup the threshold value properly. We have to make it small enough to speed-up the computation, but we should not make it too small as that can lead to inaccurate simulation results. Obviously, the threshold distance depends on all the parameters of the stress field formula. The rest of this section will use following setting of physical parameters: \( \mu = 80 \text{ GPa}, \nu = 0.31, b = 0.26 \text{ nm}, l = 30 \text{ nm}, h = 2 \text{ nm} \).

Fig 1 shows the stress field of a dipolar loop of type \( V_1 \) at several planes below and above the position of the centre of dipolar loop. It can be seen that the stress field is changing rapidly in the closest neighbourhood of the centre of the dipolar loop generating the field, whereas it vanishes fast as the distance from the loop is growing.

Let us see what we will miss if we neglect the stress field beyond some threshold distance from the centre of a dipolar loop. To get some imagination, see Fig 2 showing the stress field outside the circles of various radiuses. To be more precise, each figure shows the stress field values outside the circle of a particular radius, whereas the values inside the circle are set to zero. This allows us to compare the minimal and maximal values available at different distances from the centre of the dipolar loop. Only the plane \( z = 0 \) is showed in Fig 2 as the absolute minimum and maximum values of stress field fall down with growing distance from this plane. Hence, the other planes are not important for the idea which follows.

Tab 1 shows the minimal and maximal values of the stress field beyond the threshold distance (outside the circle of radius \( r \)). We can see that the stress field values beyond the 200 nm radius are at least 7 times smaller than beyond the 100 nm radius. However, the area of the interaction in the annulus between 200 nm and 300 nm radiuses is much larger than the area of the annulus between 100 nm and 200 nm radiuses.
Figure 2. Minimum and maximum values of the stress field beyond a circular threshold

Hence, how to pick the threshold distance properly? The idea is simple again. What error we make if we neglect the stress field in the annulus bounded between radiiuses $r_0$ and $r_1$? In fact, we are in 3D, but the dislocation curve can glide only in a slip plane. To estimate the error, we do the following. First, we assume that the maximum stress field value in the annulus is achieved in the whole annulus. Note this is a big overestimate. Second, consider the fact that the stress field of a dipolar loop interacts with segments of dislocation curve in the algorithm. The force influence would be the biggest if all the curve segments would be oriented the same (i.e. the dislocation curve would be a straight line). However, this would not fit into the annulus as the typical length of the dislocation curve is several micrometres. Therefore, assuming a circular dislocation curve inside the annulus, and ignoring the real orientations of the segments, we commit another two overestimates. The first one is that the segments are obviously not oriented the same; the second one is that though such a circular curve is rather long, it is surely not real. Nevertheless, assume a circular dislocation curve in the middle of the annulus, i.e. the length of the curve would be $2\pi(r_0 + r_1)/2$.

Using all the above information, we can evaluate upper estimates of the total force acting on a dislocation curve in the annulus (the force is generated by a dipolar loop), and, vice versa, the total force acting on that dipolar loop (as a reaction of the dislocation curve).
Table 1. Minimal and maximal values of the stress field outside of a circle around the centre of a dipolar loop, evaluated in planes $z = 0$, $z = l$, and $z = -l$.

<table>
<thead>
<tr>
<th>Threshold radius $r$</th>
<th>$z = 0$ nm</th>
<th></th>
<th>$z = \pm l$ nm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>min $\sigma_{xy}$</td>
<td>max $\sigma_{xy}$</td>
<td>min $\sigma_{xy}$</td>
</tr>
<tr>
<td>25 nm</td>
<td>-60 MPa</td>
<td>80 MPa</td>
<td>–</td>
</tr>
<tr>
<td>50 nm</td>
<td>-15 MPa</td>
<td>20 MPa</td>
<td>-15 MPa</td>
</tr>
<tr>
<td>100 nm</td>
<td>-2 MPa</td>
<td>3 MPa</td>
<td>-1.5 MPa</td>
</tr>
<tr>
<td>200 nm</td>
<td>-0.3 MPa</td>
<td>0.4 MPa</td>
<td>-0.2 MPa</td>
</tr>
<tr>
<td>300 nm</td>
<td>-0.08 MPa</td>
<td>0.12 MPa</td>
<td>-0.08 MPa</td>
</tr>
</tbody>
</table>

Table 2. Neglected force estimation in several annuluses

<table>
<thead>
<tr>
<th>$r_0$</th>
<th>$r_1$</th>
<th>Dislocation curve length</th>
<th>Force estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 nm</td>
<td>50 nm</td>
<td>250 nm</td>
<td>5.2 nN</td>
</tr>
<tr>
<td>50 nm</td>
<td>100 nm</td>
<td>450 nm</td>
<td>2.5 nN</td>
</tr>
<tr>
<td>100 nm</td>
<td>200 nm</td>
<td>1000 nm</td>
<td>0.78 nN</td>
</tr>
</tbody>
</table>

From Tab 2 it seems that the safe value for a threshold distance would be about 50 nm. 

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**References**


