MODEL VALIDATION OF A 3D SIMULATION OF DISLOCATION DYNAMICS: DISCRETIZATION AND LINE TENSION EFFECTS

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Abstract—Some fundamental aspects of 3D computer modelling of plastic flow are presented together with the results of a detailed study of related approximations, such as the discretization of space and of dislocation line curvature. More specifically, the stress field generated by different discretizations of dislocation loops and the critical stress for dislocation multiplication through the Frank–Read mechanism, are compared to the predictions of the elastic theory of dislocations in the isotropic approximation. Although crude in appearance, the approximation adopted in these simulations to describe the curvature does not drastically affect the behaviour. Moreover, it leads to critical stress values for a pinned dislocation segment in excellent agreement with previous computations.

Résumé—Afin de valider certaines des approximations fondamentales d’une simulation numérique à 3D de la plasticité, nous avons étudié l’influence du mode de discrétisation de l’espace et de la courbure des dislocations. Plus particulièrement, le champ de contrainte engendré par différentes discrétisations des boucles de dislocation, ainsi que la contrainte seuil de multiplication par le mécanisme de Frank–Read, ont été comparés aux résultats prédits par la théorie élastique en milieu isotrope. On vérifie, que le mode de discrétisation, adopté pour la courbure des lignes de dislocations, n’affecte pas de façon significative le comportement du modèle numérique. De plus, les résultats obtenus pour la contrainte critique d’instabilité d’un segment de dislocation ancré à ses extrémités, sont en très bon accord avec les résultats numériques déjà publiés.


I. INTRODUCTION

The extensive experimental and theoretical studies performed during the last five decades have substantially clarified the microscopic mechanisms controlling plastic flow in crystals. Nevertheless, the prediction of the mechanical properties of materials in terms of defect properties is still an open problem. Indeed, the conditions at which self-organized dislocation microstructures are formed, their relation to plastic flow, in particular to strain hardening properties are not understood. Beyond the difficulties inherent to a detailed description of internal stresses and of microstructural features in deformed materials, this situation stems from the non-existence of a “plastic state” functional and from the fact that dislocations, the defects carrying plastic deformation in crystals, are non-equilibrium defects. Theoretical models of plastic flow have not yielded much quantitative progress because of two types of complexity, viz. the large number of processes involved and the long range of the elastic interaction between dislocations. These reasons motivated the development of numerical simulations of plastic flow, probably the only way to overcome many of the above quoted obstacles. In a series of recent papers, Kubin et al. [1, 2] and Devincre et al. [3] presented the first 3D simulation of dislocation dynamics and interactions at a mesoscopic scale. Preliminary results showed that the tendency of dislocations towards self-organization, although not yet satisfactorily reproduced, can be accounted for in spite of the complexity of the microstructures produced during straining. Therefore, a serious hope exists that numerical techniques
may allow to achieve one important goal in materials science: the connection between microscopic and macroscopic plastic properties.

The discretization of time and space is inherent to numerical simulations and this also holds for the above mentioned 3D computer model of plastic flow. Since dislocations are linear defects, simulations involve both displacement and line-curvature discretization. These unavoidable simplifications introduce specific problems mainly related to the fact that strain fields generated by “segmented loops” differ from those of continuous loops [4]. For this reason, whatever is the mode of discretization chosen, the results of the computations crucially need to be compared to theoretical predictions.

The present work focuses on the validation of the approximations stemming from the discretization of space. Compact expressions for the computation of the forces acting on dislocation segments are derived. It is shown that, due to the adopted discretization of line-curvature, it is necessary to explicitly consider the forces related to line tension effects, in addition to the mutual interactions of segments. Despite the simplifying hypotheses implied by the discretization, the results of the simulation are shown to be still realistic. Indeed, the dependence of the critical stress \( \tau \) of a pinned dislocation segment on its length is in excellent agreement with the results of previous theoretical studies. This is an important outcome from the present work since dislocation line tension and critical stress calculations are key quantities controlling many microscopic deformation mechanisms. They must, therefore, be accurately accounted for in 3D numerical models.

The present paper is organized as follows: Section 2 presents the main ingredients used in the 3D simulation of plastic flow, as well as a description of the validation tests performed in present work. In this part are successively presented: (i) the geometrical framework; (ii) the expression of the stress field of straight dislocation segments; (iii) the calculation of the total force experienced by a dislocation segment, as a result of interactions with other segments and of line tension effects; and (iv) the minimization procedure used to determine equilibrium configurations and critical stress values for a Frank–Read source. The results obtained are presented in Section 3 and consist of a comparison of the stress fields generated by the discretized line-curvature model used in the 3D simulation with those of regular polygonal loops. The critical stress of a pinned dislocation segment is compared to the prediction of the elastic theory and to values obtained by previous computations. Finally, these results are discussed and summarized in Section 4.

2. MODEL AND COMPUTATIONS

2.1. Geometrical models

A first step, needed in setting up 3D simulations of dislocation dynamics, consists in the discretization of space. This implies both a discontinuous representation of dislocation characters and the replacement of each continuous dislocation line by a set of contiguous segments. In the present case, a very simple solution has been adopted: curved dislocations are approximated by a collection of straight segments with only two possible character, screw or edge. This is schematically shown in Fig. 1 for the case of an elliptical dislocation loop expanding in its slip plane. The underlying grid (broken lines) represents possible sites occupied by the segments during the expansion process. For f.c.c. materials, the space is tiled with a three dimensional lattice consisting of a set of \( \langle 110 \rangle \) (screw) and \( \langle 112 \rangle \) (edge) directions.

The initial configuration is a random distribution of sources, i.e. a collection of glissile dislocation segments pinned at their ends and with same density on each slip system. The elementary translation distance on this 3D lattice, has been attributed a value,
a, compatible with twice the annihilation distance, $y_a$, of edge dipoles in the considered material. Essmann and Mughrabi [5] have determined experimentally this value in copper: $y_a \approx 1.6$ nm, hence $a = 5.54$ nm [2]. The simulation box contains about $6 \times 10^9$ such cells forming a cube of side $\approx 10 \mu m$. Among various possible boundary conditions, those currently employed simulate free surfaces without accounting for image forces [3, 4]. Dislocations lines that reach the surface of the box are eliminated. A typical initial configuration, corresponding to a dislocation density $10 H m^{-2}$, is shown in Fig. 2. These basic aspects of the simulation have been already discussed in detail in [1-3] and will not be reproduced here.

One may wonder whether or not the drastic approximation of the dislocations line-curvature adopted in the simulation is still realistic. To answer this question the following validation tests were performed.

(i) The stress field generated by two models of dislocation loops, discretized according to the above procedure, are compared to the one generated by a regular, polygonal, reference loop built up with 16 segments. Indeed, Bacon and Crocker [6] have shown the latter to be an excellent approximation of a circular dislocation loop (Fig. 3). The first model corresponds to the lowest possible discretization level making use of edge and screw dislocation segments: a square loop, referred to in the following as model A (Fig. 3). The second (model B) is constructed on the basis of the reference polygonal loop (model C), by replacing each mixed segments by an appropriate combination of three edge and screw segments (Fig. 3). Equal areas were assigned to the three model loops, in order to satisfy the basic requirements of a comparison among the associated stress fields [4].

(ii) The critical stress, $\tau_c$, beyond which a pinned segment becomes unstable is computed. The variation of $\tau_c$ as a function of the segment length is determined for various discretization levels and these values are compared to the results of previous computations [7]. Since fine tension, the major property controlling the equilibrium shape of Frank-Read sources, is also involved in a large number of fundamental mechanisms, this validation test is of crucial importance for the simulation.

2.2. Stress field of a straight dislocation segment

The computation of the stress field due to an array of curved dislocations, each being approximated by a sequence of straight segments, is a standard technique [4]. Such a discretization has been successfully used to compute loop energies, the line tension or the dilatation caused by dislocation loops [8-11].

According to de Wit [12-13] the stress tensor elements, $\sigma_{ij}$, generated at a point $Y$ by a straight dislocation of Burger's vector $b$ (Fig. 4) are given, within the frame of isotropic elasticity, by

$$
\sigma_{ij} = \frac{\mu b_i}{8\pi} \left( \epsilon_{ijm} + \frac{2}{(1 - \nu)} \delta_{ij} \right)
$$

where

$$
\epsilon_{ijm} = q_{ijm} \left( \epsilon_{ijm} t_i + \epsilon_{imn} t_n \right)
$$

$$
\delta_{ij} = \epsilon_{ijm} q_{ijm} - q_{jm} q_{im}
$$

Repeated indices are summed. $\mu$ and $\nu$ are respectively the shear modulus and the Poisson's ratio, $\delta_{ij}$ is the Kronecker symbol and $\epsilon_{ijk}$ represents the permutation operator whose non-zero elements are

$$
\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1 \quad \epsilon_{132} = \epsilon_{213} = \epsilon_{321} = -1
$$

The Euclidian distance of point $Y$ to the straight dislocation, is the norm of the vector $\rho$ such that

$$
\rho = R - Lt
$$

$$
L = R \cdot t
$$

where, $R$, is the distance of one point I of the dislocation and $Y$ (Fig. 4). $q$ is given by [13]

$$
q = \int R \cdot dl
$$

and $q_{ijm}$ represents the third-order derivatives of $q$.

Equation (1) is better suited for numerical calculations than other equivalent expressions [4, 14-17] because the stress components due to individual segments can be conveniently expressed in a common reference system. For this purpose, the third-order derivatives of $q$ are needed. These quantities are not available in the literature to the authors knowledge.
they are computed in the Appendix. A simple expression for the stress tensor is obtained by defining a vector $Y$ such that

$$Y = R + Rt = (L + R)t + \rho$$

(7)

and the symmetric tensorial operator

$$[abc] = \frac{1}{2}[(a \times b)c_i + (a \times b)c_j].$$

(8)

After some algebra (cf. Appendix) one obtains the expression for the stress tensor elements generated at a point $I'$ by a straight segment $AB$

$$\sigma_{ij}(AB) = \frac{1}{2(1 - v)}(b, Y, T)(\delta_{ij} + Y_{ij} + \rho Y_{ij} + \frac{L}{R} Y_{ij}).$$

(9)

$$(b, Y, T)$$ denotes the scalar triple product and

$$\phi_y = \frac{2}{Y^2}(\rho Y_i + \rho Y_i + \frac{L}{R} Y_{ij}).$$

(10)

It is worth being noticed that in the tensorial stress expansion of equation (9), the contributions stemming from screw and edge components appear in different terms. Advantage is taken of this feature to improve the efficiency of the 3D simulation code, by dropping the terms irrelevant to each specific case. This improvement originates from the specific line-curvature discretization adopted here. Under these conditions, the computation of the stress tensor at the middle of each segment of a 3D dislocation array consisting of $N = 1500$ segments ($\approx N^2$ operations), requires approximately 1 min CPU-time on an IBM Risc 6000/730 workstation.

2.3. Total force computation

The ultimate purpose of the simulation is to study the dynamical behaviour of an initial collection of straight segments such as the one shown in Fig. 2. This task requires the computation of the total force acting on each segment as well as the detailed treatment of other interactions such as annihilation events and dislocation reactions. Since the latter have been extensively described in Ref. [18], we exclusively focus here on the former. The total force exerted on dislocation segments is composed of the three following contributions:

(i) the force due to the externally applied stress, $\sigma_0$;

(ii) the force due to the interactions of a given segment with all other segments belonging to the same dislocation or to different dislocations; and

(iii) the virtual force related to line tension which we introduce below.

Segments in the simulation box are submitted to the Peach–Koehler force [19], due to the external stress (i), and to forces arising from mutual interactions (ii), as given by equation (9). In general, the resultant force on a given segment depends on the position at which it is computed. Since the minimum segment length is fixed by the discretization of space (cf. Section 2.1), a decision has to be made about how to compute the force components arising from mutual interactions. The strategy adopted consists of summing up the contributions (i) and (ii) at the middle of the segments. Although this calculation is rigorous it may result in a poor approximation if the considered segment is displaced rigidly under the effect of the resultant force. Indeed, the resultant of mutual interactions computed at different points along a given dislocation segment can differ considerably. In such conditions there is no reason to assume that the force computed at one position is acting on the whole segment. This is nevertheless the displacement rule one has to adopt to face a twofold limitation: the need for a refinement of the discretization of space and the parabolic increase in computational task when the number of segments increases. Thus, the need for a validation of the simulation model on which this work focuses on follows from the preceding remarks.

In the computational procedure described above, a non-obvious additional contribution to the total force has been ignored, which is related to the adopted discretization rules. If a segment $S$ glides rigidly over a certain distance, under the influence of the external force, lateral segments, of length $L$, must be added in order to preserve the connectivity of the dislocation line. Depending on the initial length of $S$, the additional forces it experiences through interactions with the new segments $L$ can be vanishingly small e.g. when $S$ is large and $L$ is small. Nevertheless, the creation of lateral segments contributes to the increase of the total dislocation length and thus should exert on $S$ a virtual force, which defines the line tension [20, 21]. This can be understood by recalling that the elastic energy of a collection of finite segments is usually written as a sum of two terms, the interaction-energies and the self-energies, the latter depending on the segments lengths [8, 13]. The computation of this virtual force component goes as follows.

In the frame of our simulation model, a dislocation segment is always normal to its next neighbours.

![Fig. 5. Displacement of a dislocation segment, n, of a discretized dislocation. The displacement of segment n exclusively affects the length of its first neighbours, segments n - 1 and n + 1.](image-url)
(cf. Fig. 5). Thus, when the \( n \)th element of a discretized dislocation line moves from \( x \) to \( x + \delta x \), the resulting variation of the total self-energy only stems from change in length of its lateral segments, \( n-1 \) and \( n+1 \). The resulting virtual force, \( F^{\text{v}} \), exerted on segment \( n \), is then given by the gradient of the elastic self-energy stored into the system, as the length of the lateral segments is modified

\[
F^{\text{v}} = -\left( \nabla E_s^{(n-1)} + \nabla E_s^{(n+1)} \right)
\]

with

\[
\nabla E_s^{(n)} = \frac{\partial E_s^{(n)}}{\partial x_i} = \frac{\partial L^{(n)}}{\partial x_i} \frac{\partial E_s^{(n)}}{\partial L^{(n)}}
\]

\( x_i \) (\( i = 1-3 \)) is the displacement vector and \( E_s^{(n)} \) is the self-energy of the segment \( n \), of length \( L^{(n)} \). It follows from the adopted geometry that the relation \( \partial L^{(n)}/\partial x_i = \pm 1 \) is always valid. Finally, \( F^{\text{v}} \) is calculated with help of equation (11), taking the derivative of de Wit's expression [13] for \( E_s^{(n)} \)

\[
\Delta E_s^{(n)} = \frac{\partial L^{(n)}}{\partial x_i} \frac{\mu b^2}{4 \pi (1 - v)}
\]

\[
\times \left[ \left( \frac{1}{8} - \frac{1}{2(v-1)} \right) \left[ b^2 - v(b \cdot t)^2 \right] \ln \left( \frac{2L^{(n)}}{r_0} + 1 \right) \right] \times \left[ \frac{1}{8} - \frac{1}{2(v-1)} \left[ b^2 - v(b \cdot t)^2 \right] \right]
\]

Equation (13) is expressed in a reference frame of axes \( X \), \( Y \) and \( Z \) parallel respectively to the direction of the considered segment, to the glide direction and to the normal to the glide plane. Other contributions to the total force exerted on each segment are also resolved into this system of axes. This local reference system will be used throughout the present work. It is worth noticing that equation (11) only involves contributions from next-neighbouring segments. Thus this “line-tension” force is by nature short-ranged as opposed to the long-range elastic interactions of the segments.

2.4. Displacement rules and minimization procedure

To find out the equilibrium configuration of a dislocation segment pinned at its ends and submitted to an external force, one can either minimize the total elastic energy or the effective forces acting on the dislocation loop with respect to its shape. The last approach is adopted in present work, as it is naturally suited to the 3D simulation. The minimization procedure is performed as follows.

(a) Given an initially straight dislocation segment of length \( L \), pinned at its extremities, the discretization level is defined by fixing arbitrarily the maximum number of edge and screw subsegments into which it will be subdivided under the action of the external force. The length of these subsegments is initially set to zero; it evolves during the minimization process. The new coordinates at time \( t + \delta t \), \( x(t + \delta t) \), are then given by

\[
x(t + \delta t) = 2x(t) - x(t - \delta t) + \frac{\mathbf{F} \delta t^2}{m^*}
\]

\( \mathbf{F} \) is the total force per unit length acting on a subsegment, and \( m^* \) is a virtual mass associated to the subsegments. All the displacements take place along the glide direction of the subsegments. After each step, subsegments are added, if necessary, up to the maximum number \( N_e \) allowed by the chosen discretization level. In addition, the length of the subsegments adjacent to those which have moved is modified in order to preserve the connectivity of the expanding dislocation loop.

(b) An initial set of displacements is computed for all the subsegments of non zero length, with help of the usual central difference algorithm. The new coordinates at time \( t + \delta t \), \( x_i(t + \delta t) \), are then given by

\[
x_i(t + \delta t) = x_i(t) - \frac{\delta x_i}{\delta t}
\]

\( \delta t \) and \( m^* \) are adjusted so that equation (14) yields displacements that converge cannot be obtained. Therefore, the computed displacement values are converted to the nearest integer value, chosen in the range 1 to 10 lattice constants. The values of \( \delta t \) and \( m^* \) are adjusted so that equation (14) yields displacements within the defined range.

This procedure is similar in its spirit to the quasidynamic minimization algorithm used in atomistic simulations [22]. When equilibrium is approached, the frequency at which displacements are accepted decreases. Convergence is considered to be effective when none of the displacements computed via equation (14) is accepted over a hundred successive attempts. In a typical minimization about \( 4 \times 10^3 \) steps are sufficient, whatever the partition level.

3. RESULTS

3.1. Stress field of polygonal dislocation loops

The three loop models considered, viz. A (square loop), B (polygonal loop of 28 segments built according to the discretization rules of the simulation) and C (16 sides-regular polygonal loop), have the same area. The stress fields generated by these loops have been computed as a function of the distance along the two directions labelled 1 and 2 in Fig. 3. Both directions are contained in the glide plane: axis 1 is parallel to the glide direction of the edge segments while direction 2 is at \( \pi/4 \) of axis 1. This choice is dictated by the fact that the largest discrepancies between stress values generated by the model loops are found along these directions. The calculation is performed with the value \( \nu = 0.44 \) for the Poisson’s ratio. Reduced units are used: \( r^* = r/r_0 \) for distances, where \( r_0 \) is the radius of a circular loop having the same area as that assigned to the model loops and \( \sigma^* = \sigma (\mu b \sqrt{r}) \) for the stresses.
Figure 6 shows the variation of $\sigma_{xz}$, the unique nonzero stress component along direction 1, as a function of the radial distance from the centre of the loop. By comparison to our reference (model C), model B behave satisfactorily since the stress values converge rapidly with distance to the reference values. By contrast, model A yields substantially different values at short distances. This is an expected result according to a previous work by Kroupa [23]. This author has shown that for radial distances shorter than twice the loop radius, large discrepancies exist between the stress field generated by model A and the prediction of elastic theory for a circular loop. However, beyond this distance, the values of $\sigma_{xz}$ for the square loop differ by less than 10% from the exact values.

The results obtained along direction 2 are shown for $\sigma_{xy}$ alone, (cf. Fig. 7), since the variation of $\sigma_{xy}$ is much similar to that of Fig. 6. The stress component $\sigma_{xy}$ is originated from the finite length of dislocation segments considered in this work; it vanishes in the case of an infinite straight dislocation [4]. Again, model A yields significant discrepancies with respect to the reference loop. Further, one can see from Fig. 7 that the sign of $\sigma_{xy}$ inside the loop, is reversed with respect that of the reference loop. By contrast, model B behaves satisfactorily, especially at distances large compared to the loop radius, although higher order partitions are still needed to improve the results at short distances.

3.2. Critical stress

The results presented in the previous section show that by refining the partition, the stress field of the discretized dislocation loops converges to that of the reference model. For a given partition, the question arises of how the critical stress $\tau_c$ above which a pinned dislocation segment becomes unstable, compares to the elastic theory prediction. The computation of the critical stress has been performed by using the quasidynamic minimization procedure detailed in Section 2.4 applied to the following three parameters: the initial segment length, its character, edge or screw, and different partitions corresponding to $N_d = 5, 9, 13, 17$ and 37 segments. The critical stress is identified as the resolved stress $\tau_c$, at which the minimization procedure fails to find an equilibrium position for the bowed out dislocation.

The calculated dependence of $\tau_c$ on the number of subsegments is shown on Fig. 8 for a segment of initial length $L = 21000 \, b$. This value of $L$ is characteristic of the initial dislocation distributions used in the 3D simulation [3]. $\tau_c$ rapidly converges towards a value identical to that given by Foreman [7] and based on a calculation involving subsegments of mixed character. Partitions containing more than 15 segments can practically be considered as having converged to Foreman's values, all the more as the segments move on a discrete lattice, which limits the accuracy. Open data points on Fig. 8 represent the values obtained when interaction forces are neglected. This clearly shows that line tension accounts for approximately 80% of the theoretical critical stress value.

The more realistic case of a pinned dislocation segment with side arms leads to critical stress values lower than those reported here [7, 24]. We have not
considered this case since our main goal is to establish the limitations inherent to the discretization modes used in the 3D simulation. However, the above remark implies that a realistic initial condition for the simulations should include Frank network, with triple nodes, rather than a distribution of sources. In addition, the stress fields of dislocation segments used in the present work are, strictly speaking, not valid for dislocation lines ending abruptly inside the crystal.

The dependence of the critical stress of a pinned segment on its initial length is given in Fig. 9. The partition level is $N_d = 17$, a value sufficiently large to ensure that discretization introduces no artefact, as shown above. In Fig. 9, $\tau_0$ and $L$ are expressed in units of $\mu b / L$ and $b$, respectively. One can see that the expected logarithmic dependence of the critical stress [7]

$$\tau_0 = \frac{A}{2\pi} \left( \frac{\mu b}{L} \right) \left( \log \left( \frac{L}{r_0} \right) + B \right)$$

(15)

is recovered. Where $r_0 \approx b$ is the core radius, $A$ takes the values 1 and $1/(1 - v)$ for screw and edge segments respectively and $B$ represents the contribution of the dislocation environment to the interaction terms [7]. In a line tension model calculation for a pinned dislocation segment without side arms, $B$ is usually set to zero. Side arm effects have been discussed by Bacon [24] and Foreman [7] who showed that they contribute to $\tau_0$ by no more than a few percent. This is equivalent to a small change in $B$ in equation (15). For this reason, such effects have not been considered in more detail. The logarithmic dependence of $\tau_0$ on the length $L$ is entirely due to the line tension contributions to the total force acting on each segment. Indeed, calculations including only mutual interactions, lead to a linear dependence of the critical stress on $L$.

The fairly good agreement of our calculations given in Fig. 9 with the results of Foreman [7], validates our approach despite the apparent roughness of the approximations involved. The computed equilibrium shapes exhibit a close similarity to those deduced from the elastic theory. Dislocation segments bowing under the action of an applied stress adopt elliptical equilibrium shapes which minimize the elastic energy. This is a manifestation of the difference in the contributions of edge and screw dislocations and the curvature adopted at equilibrium reflects this anisotropic behaviour. Figure 10 shows that the discretized dislocation models also reproduce this subtle feature. Therefore, one is further reinforced in considering that the specific space and dislocation curvature discretizations used in the 3D simulation of plastic flow are reasonably safe.

4. DISCUSSION AND CONCLUDING REMARKS

The main goal of the present work was to validate the basic assumptions of a 3D simulation of dislocation dynamics by using well established results of the elastic theory of dislocations as a guide. For the sake of simplicity, our study is confined to the framework of the isotropic approximation of linear elasticity. A more realistic approach could include elastic anisotropy effects. However, elastic anisotropy is not thought to be a relevant factor as far as collective dislocation properties are concerned, especially in f.c.c. metals and alloys.

In the same way, a possible influence of the friction force [24] has not been considered here since the friction forces used in the 3D simulation of f.c.c. crystals are fairly small.

The dependence of the critical stress on the partition level shown in Fig. 8 may be erroneously interpreted as authorizing the crudest possible approximation of line-curvature, i.e. the square loop model (model A). Indeed, the discrepancy existing in
this case between theoretical and computed values may appear acceptable regarding the gain in computational efficiency obtained when the total number of subsegments is decreased. Unfortunately, it is also shown that the stress field generated by a square loop is largely unrealistic (cf. Figs 6 and 7). Thus, the internal stress produced by a spatial distribution of such loops should be incorrect. This problem is naturally by-passed in 3D simulations, since forest dislocations prevent the formation of square loops. Then, the internal stress rather results from the superposition of the stress fields of dislocation segments pinned at junctions formed with the forest dislocations.

Finally, two features have to be considered referring to possible configurations of dislocations dynamically produced by the simulation: (i) core effects at small interaction distances and (ii) the interactions of two colinear segments. Core interactions do not occur thanks to the discretization in space and to explicit simulation rules which preclude the simultaneous occupancy of lattice sites by two segments. In the case where a contact interaction is to take place between two segments, the possible reaction is anticipated by the rules of the simulation and treated through appropriate rules [18]. In the case of two colinear segments, the computation of interaction forces is performed not in the middle of each segment but slightly apart from their common line, thus avoiding computational divergencies.

In conclusion, we have shown that the main approximations present in the present version of the 3D simulation, namely spatial and line-curvature discretization, do not significantly affect the stress field generated by dislocation loops provided appropriate partition level is chosen. Similarly, the critical stress of pinned dislocation segments is in excellent agreement with the predictions of the classical elastic theory. 3D simulations of plastic flow are of incomparably more realistic than existing 2D simulations. The latter cannot, for instance, treat line tension effects and their consequences, in particular dislocation multiplication, nor the interaction of the screw and edge parts in an expanding loop. However, the complexity arising from the number of elementary mechanisms that have to be accounted together with the occurrence of some unavoidable approximations request extensive validation. This is the motivation of present and ongoing work.

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APPENDIX

According to de Wit [13] the integral in equation (6) is written

\[
q = \int R dL = -\frac{1}{2} \mu \left[ \ln(L + R) - \frac{1}{2} LR \right]
\]  

(A1)

and the corresponding second order derivative is:

\[
q_{ij} = -\frac{\delta_{ij} - t_{ij}}{R} \ln(L + R) - \frac{\rho_{i} t_{j}}{R(L + R)} + \frac{\rho_{j} t_{i}}{R(L + R)} - \frac{\rho_{i} \rho_{j}}{R(L + R)}
\]  

(A2)

Accordingly, one obtains

\[
q_{mm} = -2 \frac{Y_m}{R(L + R)}
\]  

(A3)

Since by definition

\[
e_m t_m = (t \times t) = 0
\]  

(A4)

the general expression for the third order derivative is

\[
q_{mnn} = \frac{(R_m + R_n)}{R(L + R)} \left( \frac{\delta_m t_n + \delta_n t_m}{R} + \frac{\rho_m t_n + \rho_n t_m + L t m t n}{R^2} \right) \rho_m - \frac{\delta_m \rho_n + \rho_m \rho_n}{R(L + R)} + \frac{\rho_m \rho_n}{R(L + R)^2} \rho_m \left( 2 \frac{L}{R} \right)
\]  

(A5)
With help of equations (A3) and (A5), the stress tensor elements of equation (1) of the text are obtained. The notation is greatly simplified by introducing the tensor operator defined by equation (8) and the mixed product $(b, p, t)$.

Finally, equation (9) is derived from equation (A6) with help of the following relations

\[ (b, p, t) = (b, Y, t) \quad (A7) \]

and

\[ Y^2 = 2L(L + R). \quad (A8) \]

\[
\sigma_{ij} = \frac{\mu}{4\pi R(L + R)} \left\{ \frac{(b \times Y)_{ij} + (b \times Y)_{ji} - \frac{1}{(1 - v)}[(b \times t)_{ij}Y_{j} + (b \times t)_{ji}Y_{i}]}{\delta_{ij} + t_{ij} + \frac{(\rho_{ij} + \rho_{lj} + \rho_{lj} + \rho_{lj})(L + R)}{R^2} + \frac{2 + L}{R(L + R)}} \right\}. \quad (A6)
\]