Mat. Res. Soc. Symp. Proc. Vol. 653 © 2001 Materials Research Society

New Line Model for Optimized Dislocation Dynamics Simulations

Ronan Madec, Benoit Devincre and Ladislas P. Kubin
Laboratoire d'Etude des Microstructures,CNRS-ONERA,
29 Av. de la Division Leclerc, B.P. 72, 92322 Ch tillon Cedex, France.

ABSTRACT

A new model for the discretisation of dislocation lines is presented, which is optimised for mesoscale simulations of dislocation dynamics. By comparison with the existing "edge-screw" model, the present one provides a better description of the stress field close to the dislocation lines. It simplifies the modelling of dislocation reactions and accelerates computations by allowing to make use of larger time steps. An application to attractive junctions and forest hardening is briefly sketched.

INTRODUCTION

Ten years ago the first three-dimensional mesoscopic simulation of dislocation dynamics (DD) was proposed [1]. In the latter, a simplified description of dislocation core properties was combined with an elastic frame in order to model the dynamics of dense dislocation microstructures. The most noticeable aspect of this model was the geometrical solution proposed to discretise the dislocation lines [2]. Indeed, for the sake of computing efficiency, it was proposed to replace the continuous lines by a succession of discrete segments with edge and screw characters. This "edge-screw" simulation has been successfully used to study plastic deformation in different types of crystals, hence demonstrating its versatility (see ref.˚[3] for a short review). More recently, it has been coupled with a finite element code in order to deal with complex boundary value problems and/or complex loadings [4-5].

Other three-dimensional DD simulations have been developed in the past years [6-8]. They differ from the "edge-screw" model mainly in their geometrical formulation. The decomposition of a segment length and character is not performed on a finite set but in the continuum, in order to reproduce the line curvature as closely as possible. In spite of some technical complexities, this approach has the ability of better reproducing the elastic field close to the dislocation lines.

Whatever the geometrical model considered, the computations have been restricted up to now to relatively small simulated volumes ~$(15\mu m)^3$ and plastic strains (<1%), mostly because of two critical issues. First, the CPU requirement for DD simulations increases extremely fast with the number of interacting segments yielded by the discretisation. The use of algorithmic solutions that reduce such dependence has alleviated but not removed this difficulty. Secondly, many degrees of freedom must be updated along the moving lines and the elementary time steps can be fairly small in materials with high dislocation mobility. As a result, quasi-continuous models favour a reduction of the number of segments per unit line length, whereas fully discretised models favour larger time steps. Thus, a compromise between the two types of discretisations should yield an optimum efficiency.

A modified version of the "edge-screw" model, the "edge-mixed-screw" model, is presented here, which includes two additional characters per slip system. The improvement thus obtained is briefly discussed and illustrated by validation tests. An application is presented to the treatment of dislocation junctions.

DISLOCATION DISCRETIZATION

To preserve the advantages of the "edge-screw" model, the latter has been modified by adding new directions into the finite base of vectors used to discretise the dislocation lines and their displacement steps [1]. These mixed directions, ξ_m, are defined as linear combinations of the edge and screw vectors, i.e., $\xi_m = n\xi_s + m\xi_e$.

As illustrated by Figure 1, the simplest modification consists of adding two 60¡ directions (n, m = –1) per slip system. This solution was found to give satisfactory results in several respects. i) - It does not involve drastic changes in the"edge-screw" model. ii) - It provides an improved description of the dislocation self-stress field (cf. Figure 3 of [9] for a detailed discussion). iii) - It significantly reduces the number of segments required to model a given dislocation microstructure. This last improvement is particularly important for such frequently met configurations as dipoles of arbitrary line orientation and junctions. For instance, as shown in Figure 2 for the case of f.c.c. crystals, the possible directions of the Lomer locks are parallel to either the screw or mixed direction (their character being either edge or mixed) and can be modelled with very few segments.

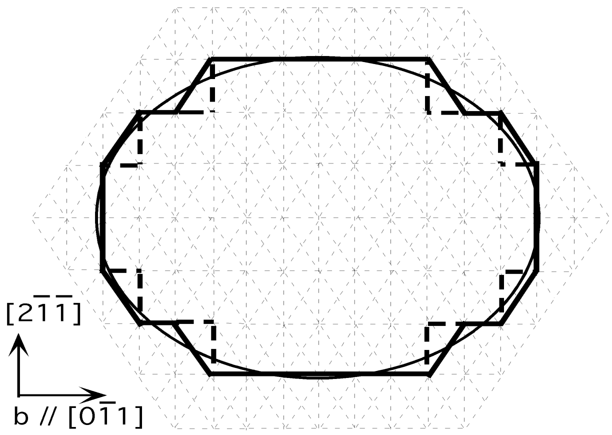


Figure 1*. Modelling a small dislocation loop by the "edge-screw" line model (dotted lines) and the "edge-mixed-screw" line model (bold lines). The latter involves both a reduced number of segments and a better description of the continuous shape. The figure is drawn for a (111) slip plane in an f.c.c. crystal, with a Burgers vector b parallel to the $[0\bar{1}1]$ direction.*

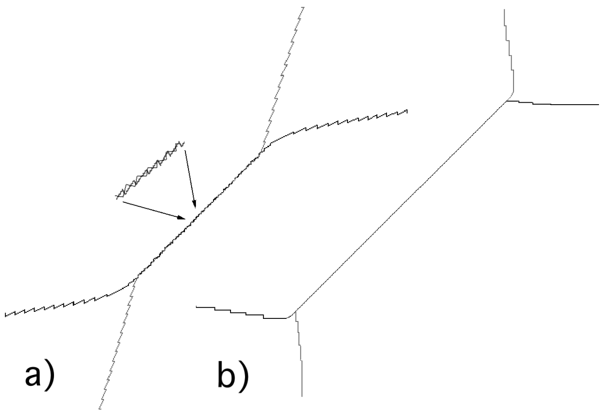


Figure 2*. A relaxed junction between two dislocation lines treated with (a) - the "edge-screw" model and (b) - the "edge-mixed-screw" model. In (a), more than 50 segments are needed to obtain an accurate description of the junction line, whereas 2 segments only are sufficient in (b). Notice that the line tension equilibrium at the triple nodes is better achieved at short distances in (b) due to the better description of the line directions.*

In addition, the use of edge, screw and – 60¡ characters is of interest for the treatment of the lattice friction or Peierls stress when they are significant. In such cases, dislocations slip occurs by a kink-pair mechanism and results at the mesoscale in the motion of straight and rigid lines parallel to dense atomic rows. This applies typically to the screw line directions in b.c.c. crystals, the screw and – 60¡ directions in diamond cubic crystals and the screw directions in the {111} slip planes of $L1_2$ alloys.

DISLOCATION DYNAMICS

The modifications brought into the simulation do not affect the parts of the code devoted to the calculation of the internal stresses and the integration of the equations of motion. They induce an increase of the time spent in the computation of the interaction stresses by about 50%. This extra computing time stems from the relative increase, in the new line model, of the number of non-screw segments, whose stress field is more complex than that of screws. However, due to the decrease in the total number of segments, the net result is an overall decrease in computing time.

The constitutive rules that maintain the connectivity of the segments during their displacement, as well as the procedures for the discretisation of dislocation line curvatures are not significantly altered. The main changes are due to the fact that the length of a segment is now modified during its displacement. This is not the case with the "edge-screw" model, since the segments always move along a direction parallel to that of their neighbours. As a result, the algorithm dealing with the search of obstacles (e.g., forest dislocations, precipitates, interfaces,) in the swept area becomes more complex. Nevertheless, most of the related procedures can still be tabulated.

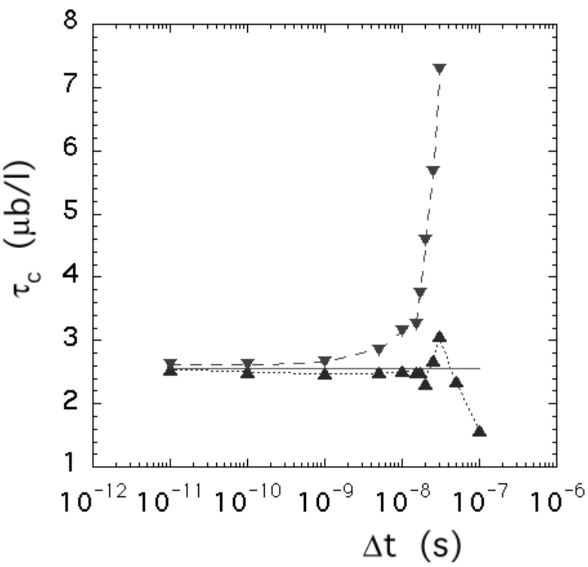


Figure 3*. Simulation of the critical stress of a Frank-Read source in copper (in units of μb/L, where L is the length of the source segment, of screw character, and μ the shear modulus) as a function of the time step. The domain where a good agreement between theory (continuous line, after Foreman [10]) and simulation is obtained extends to larger time step values with the "edge-mixed-screw" model (upwards triangles) than with the "edge-screw" model (downwards triangles). In the present case, the new line model allows increasing the time step value and speeding up the simulation by one order of magnitude.*

Altogether, this part of the simulation is significantly accelerated not only because of the reduction in the number of segments but also due to the increase in the time step value. This last important result is illustrated by Figure 3 and has two origins. First, the discretisation leads to smoother shapes and smaller fluctuations in the local line tension. Hence, this allows making use of larger elementary displacements. Secondly, with a smaller number of segments, the number of degrees of freedom per unit line length is decreased. As a consequence, the occurrence of parasite transversal wave modes along the lines is strongly reduced.

CONTACT REACTIONS

The "edge-mixed-screw" model also provides a better description of the dislocation stress field close to the lines. This improves the quantitative aspects of the simulations, particularly regarding the modelling of contact reactions. For instance, in the "edge-screw" formulation, some local rules are commonly used to help implementing the formation and destruction of junctions [11]. These phenomenological rules are useful to by-pass a detailed description of the junction geometry, as the latter requires, a substantial amount of small segments (cf. Figure 2) and a small time step (cf. Figure 3). Such simplifications are no longer necessary with the "edge-mixed-screw" model and the junction properties can be treated without approximation. The problem of dealing with the equilibrium configuration of junctions is then reduced to a simple question of force balance at the triple nodes. The corresponding validation tests are given in the next section. For the same reasons, the new line model allows performing a better treatment of the short-range interactions with any type of elastic defect. Finally, if the use of the – 60¡ mixed directions is well suited for treating junctions, different line directions could be preferred for dealing with other specific problems. For instance, when treating plastic deformation in the vicinity of an interface, it could be advantageous to introduce segments parallel to the latter.

JUNCTION PROPERTIES

From the numerous previous investigations carried out in the early days of dislocation theory (see e.g. [12, 13]), it was concluded that the formation and destruction of junctions constitutes the major contribution to strain hardening. Further, it was shown that junctions are basically low energy configurations whose main properties can be predicted with the help of simple elastic arguments involving a simplified formulation of the line energy.

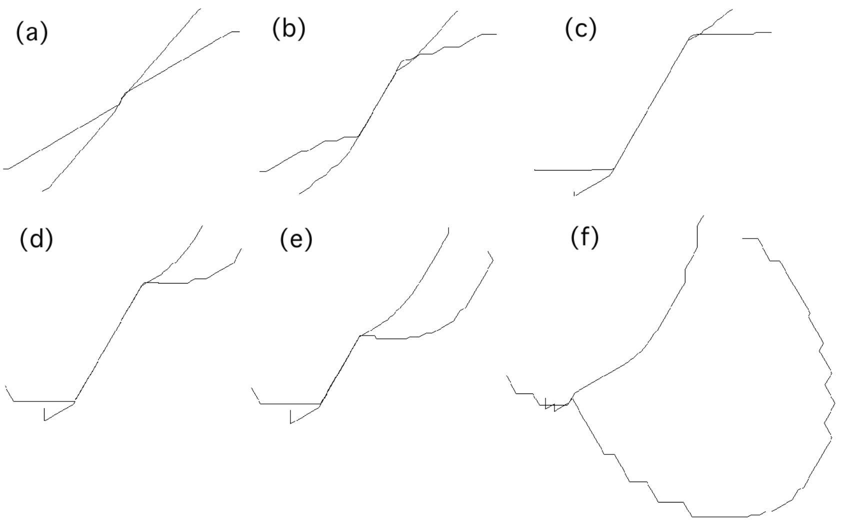
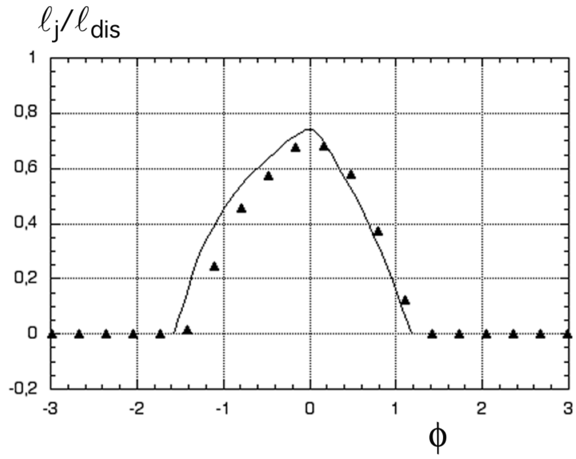
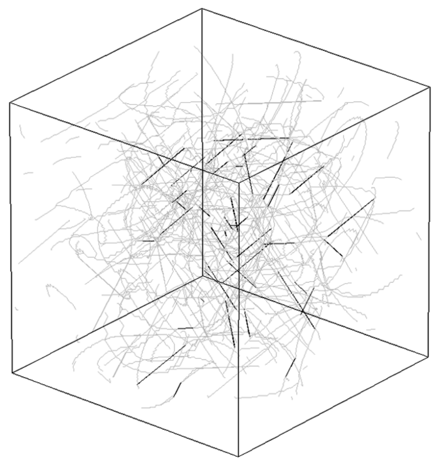


***Figure 4**. (a) - (c): Zipping of a junction in the absence of applied stress and under the effect of the elastic interactions between the two attractive segments. (d) - (f) : Unzipping of the same configuration under stress. The two interacting slip systems are $1/2[\bar{1}01](1\bar{1}1)$ and $1/2[1\bar{1}0](11\bar{1})$.*

This last result was confirmed by more recent calculations, both at atomic and mesoscopic scales [14-16]. Detailed checks have been performed on the "edge-mixed-screw" model and are illutrated by Figures 4 and 5. Figures 4-a to -c show the zipping of a junction under zero stress from two attractive segments which cross each other at their mid-point. The sequence of Figures 4-d to -f shows the unzipping of the same configuration under stress. From such tests, one can derive a mapping of the various possible configurations, of the junction lengths and the critical stresses for junction unzipping as a function of the initial orientation of the segments [16]. For instance, Figure 5 shows the simulated junction length when the orientation of one segment is fixed to an angle ϕ_o = - 0.47 rad. with respect to the $[0\bar{1}\bar{1}]$ junction direction, whereas the other angle ϕ is let to vary. Junctions of different lengths ℓ_j are formed within a range of values of the angle ϕ. The slight asymmetry of this domain is due to the dependence of the self-energy on dislocation character. For large values of ϕ, either repulsive configurations or attractive configurations that do not form junctions (crossed-states) are obtained. The excellent agreement obtained with respect to a simple elastic model (see ref. 15 for detail) confirms that the "edge-mixed-screw" model can realistically treat junction properties.



Figure°5. *Junction length ℓ_j, reduced by the initial length of the segments ℓ_{dis}, as a function of the orientation ϕ of one of the segments, the other one being fixed. The data points show the simulation results. The full line is a prediction obtained from a balance of energy involving a simplified line energy model.*



Figure°6. *A multiple slip configuration obtained with a [100] stress axis in a simulated box of dimension (15 µm)^3. The junction lines are shown in black and the dislocation lines in grey.*

The modelling of "forest" hardening involves performing a global average over the strengthening effect of all the junctions present in a model crystal (cf. Figure 6). In a mass simulation, the various junctions formed differ not only by several geometrical parameters (Burgers vector, slip plane, length and orientation of the lines, position of the intersection point) but also by their frequency of occurrence. For instance, one can see from Figure 5 that the configuration involving a segment parallel to the incipient junction line (ϕ = 0) produces a junction of maximum length. This configuration relaxes a maximum of elastic energy and exhibits maximum stability under stress. However, it only occurs for one particular geometry.

A global check of the new line model can be performed by investigating from mass simulations the well-known scaling law that relates the flow stress τ to the square root of the forest dislocation density, ρ_f : $\tau = \alpha\mu b\sqrt{\rho_f}$, where α is a coefficient whose value is about 0.3-0.4 in f.c.c. crystals [17]. Preliminary simulation results yield a value $\alpha = 0.38$ that falls within the expected range. These numerical experiments deserve a careful discussion, which is postponed to a further publication.

CONCLUSION

The "edge-mixed-screw" line model provides an interesting compromise between an increased computing efficiency and a better description of the dislocation fields. Through a self-consistent elastic treatment of dislocation reactions it will allow quantitative simulations of forest and strain hardening to be performed.

REFERENCES

1. L P. Kubin, G. Canova, M. Condat, B. Devincre, V. Pontikis and Y. Br chet, Solid State Phenomena, **23-24**, 455 (1992).
2. B. Devincre and M. Condat, Acta metall. mater, **40**, 2629 (1992).
3. B. Devincre and L. Kubin, Mat. Sci. Eng., **A234-236**, 8 (1997).
4. M. Fivel, M. Verdier and G. Canova, Mat. Sci. Eng., **A234-236**, 923 (1997).
5. C. Lemarchand, B. Devincre, L. Kubin and J.L. Chaboche, MRS Symp. Proc., **538**, 63 (1999).
6. H. M. Zbib, M. Rhee, and J.P. Hirth, Int. J. Mech. Sci. **40**, 113 (1998).
7. K. W. Schwarz, J. Appl. Phys. **85**, 108 (1999).
8. N. M. Gohniem and L. Z. Sun, Phys. Rev. B 60, 128 (1999).
9. B. Devincre, L. P. Kubin, C. Lemarchand and R. Madec, Mat. Sci. Eng. A, in press.
10. A. Foreman, Phil. Mag. 15, 1011 (1967).
11. B. Devincre and L.P. Kubin, Modelling Simul. Mater. Sci. Eng. **2**, 559 (1994).
12. G. Saada, Acta metall. **8**, 841 (1960).
13. G. Schoeck and R. Frydman, Phys. Stat. Sol. (b), **53**, 661 (1972).
14. V. B. Shenoy, R. V. Kukta and R. Phillips, Phys. Rev. Lett. **84**, 1491 (2000)
15. L.K. Wickham, K. Schwarz and J. S. St lken , Phys. Rev. Lett. **83**, 4574 (1999).
16. R. Madec B. Devincre and L. P. Kubin, Comp. Mat. Sci., in press.
17. J. Gil Sevillano, in H. Mughrabi (Ed.), Plastic Deformation and Fracture of Materials (Materials Science and Technology, Vol. 6), VCH, D-Weinheim, p. 40 (1993).