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

Periodic Boundary Conditions for Dislocation Dynamics Simulations in Three Dimensions

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ABSTRACT

This article presents an implementation of periodic boundary conditions (PBC) for Dislocation Dynamics (DD) simulations in three dimensions (3D). We discuss fundamental aspects of PBC development, including preservation of translational invariance and line connectivity, the choice of initial configurations compatible with PBC and a consistent treatment of image stress. On the practical side, our approach reduces to manageable proportions the computational burden of updating the long-range elastic interactions among dislocation segments. The timing data confirms feasibility and practicality of PBC for large-scale DD simulations in 3D.

INTRODUCTION

Treatment of boundary conditions is an important element of Dislocation Dynamics (DD) methodology. There are two distinct classes of DD simulations that necessitate different approaches to boundary conditions. When the simulation volume is close to an internal or external interface (surface, crack, grain or phase boundary, etc.), it is necessary to account for stress variations associated with the interface. In other cases, dislocation behavior in the bulk single crystal, far removed from any interfaces, is of interest. The first case is generally difficult requiring the use of sophisticated numerical methods [1,2] to calculate the elastic (image) stress associated with the interfaces. In the second case, the material volume can be regarded as a small part of an infinitely large single crystal justifying the use of the relatively simple analytical solutions of the continuous theory of dislocations obtained for the infinite elastically homogeneous solid [3].

Understandably, in the early stages of development, DD simulations focused on the simpler case of bulk single crystals. Many years ago von Karman suggested a trick by which a small representative volume of material is replicated by periodic continuation to make up the infinite crystal and to preserve its translational invariance. Since then, this trick has been routinely employed in computer simulations of solids. In 2D, where dislocations appear as point objects carrying tensorial (Burgers) charges, periodic boundary conditions (PBC) have been successfully implemented [4,5]. However in 3D, the models used for DD simulations in the bulk remain inconsistent with the absence of material interfaces and translational invariance of the infinite crystal. In fact, most simulations performed so far employ free boundaries. To simplify the treatment, the boundaries are allowed to exist only in the sense that they absorb dislocations that happen to approach the boundary, whereas the image stresses induced by the free surfaces are simply ignored [6]. In order to mitigate such undesirable effects, a smaller spherical volume in the center of the simulation box is sometimes used to control the loading conditions and to monitor dislocation behavior [2]. Unfortunately, the spurious dislocation loss can not be fully prevented even using such an embedded sphere approach. Furthermore, the remainder of the

simulation volume (~ 80%) is wasted because its only function is to buffer the central sphere from the free surfaces. Mirror reflection approach developed in [7] addresses the problem of image stress but the spurious loss of dislocation to the boundaries remains an issue. Recently, free surface boundary conditions have been augmented with a procedure that monitors the rate of dislocation loss to the boundaries and re-introduces dislocations at random, to counter the loss [2,8]. Although these modifications offer significant improvement over the use of plain free surface boundary conditions, the fact remains: all of them contain some sort of boundaries thus violating the translation invariance and, except for [7], ignore or distort the image stress fields associated with the boundaries.

At a first glance, an extension of PBC to 3D appears very appealing since, by their very nature, PBC preserve translational invariance and balance dislocation fluxes in and out of the box. Countering such warm feelings for the von Karmann's trick are the warnings against the use of PBC in 3D given in the earlier papers on the DD methods [6,9]. Subsequent publications reinforce the early doubts suggesting that line connectivity can not be preserved in 3D PBC [2,7, 10]. This contribution is intended to dispel the doubts and to clear the PBC for use in DD simulations in 3D. In the following we show that consistent application of PBC in three dimensions is not exactly trivial, yet its potential advantages should convince those in doubt that PBC is a good alternative to the other types of boundary conditions currently in use.

NUMERICAL IMPLEMENTATION

In this section we consider three aspects of periodic boundary conditions relevant for practical numerical implementation: (1) line connectivity, (2) initial dislocation arrangements compatible with PBC and (3) treatment of image stress.

Line connectivity

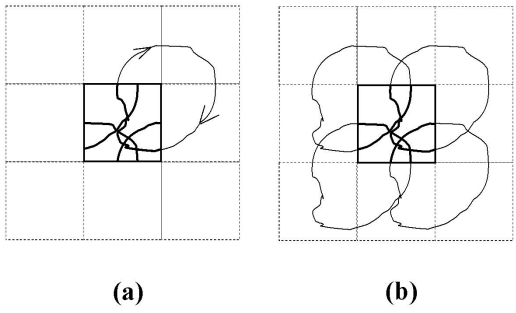

Fig. 1 *Closed loops in PBC: in (a) the primary loop (thin line) is folded in the primary box (thick line) whereas in (b) the same result is obtained by periodic loop replication.*

That there is really no problem maintaining line connectivity in PBC is illustrated in Fig. 1 that shows a closed loop of arbitrary shape partly contained in the primary box. The box is periodically replicated in 2D (only a few relevant replicas are shown for clarity). Periodic replication of the loop demands that, every time the line crosses the imagined boundary of the primary box or any of its replicas, another line enters the primary box at the periodically equivalent position on an appropriate face. By tracing the primary loop along its contour direction, one can "fold" the entire line in the primary box. To complete the periodic continuation, such folded lines are replicated in all other boxes as well. Alternatively, the same periodic arrangement of loops and boxes can be obtained without ever tracing and folding the primary loop, by simply replicating the whole loop with the same periodicity vectors as used for replicating the primary box (Fig. 1(b)). Although the illustration is 2D, exactly the same folding and replication procedures apply in 3D.

The fact that folding and replication are equivalent can be used constructively in a numerical implementation. In particular, instead of tracing the events of boundary crossing within the primary box, the algorithm can focus on the unfolded primary loop spanning many periodic boxes but perform the arithmetic manipulations with the vectors *modulo periodicity vectors*. From this point of view, there are no boundaries to deal with in the periodic boundary conditions, since the origin of periodic replication can be arbitrarily shifted with respect to the primary loop. Translational periodicity of PBC is not only physically realistic but also numerically convenient.

That line continuity is maintained in DD simulations is proven by simple induction: starting from an initial configuration such as shown in Fig. 1, line continuity is preserved in all subsequent topological transformations, e.g. recombination, multiplication, junction reactions, etc.

Initial conditions

One likely reason for the persistent prejudice against using PBC in 3D is not appreciating the fact that, when it comes to translational periodicity, not all dislocation arrangements are created equal. In fact, general dislocation configurations in the primary box can not be periodically continued in all directions without breaking the lines, however similar they may look to the one shown in Fig. 1. The latter is compatible with PBC but, having been constructed by folding a closed loop into the primary box, is by no means arbitrary. In addition to closed loops, infinite dipoles can be used to generate PBC-compatible initial configurations[1]. In this case, it is necessary to make sure that each line of the dipole eventually re-enters itself so that its total span (the vector connecting its two ends) is a multiple of the periodicity vectors. We have developed a simple algorithm of self-correcting random walk by which a line spanning a given multiple of the periodicity vectors can be generated using a sequence of random numbers. Although the class of PBC-compatible initial configurations may appear rather narrow, this is not a serious constraint for large-scale DD simulations.

It is interesting to note that all PBC-compatible dislocation configurations correspond to a net zero integral over the primary box of the so-called dislocation density or Nye's tensor [11]

$$\boldsymbol{\alpha} \equiv \frac{1}{V}\int_L \mathbf{b}\otimes\mathbf{t}\,ds = 0 \ , \qquad (1)$$

where **b** is the Burgers vector, **t** is the line tangent vector, *ds* is an element of arc length along the dislocation line, and *L* is the total length of dislocation lines within box volume *V*. For our purposes the integral is conveniently reduced to a simpler form [12]

$$\alpha_{ij} \equiv \frac{1}{V}\sum b_i (x_j^+ - x_j^-) = 0 \ , \qquad (2)$$

where x^- and x^+ are the positions of entry and exit points of the line segments and the sum includes all dislocations inside the box.

Although the condition of zero Nye's tensor integral is realized for all initial configurations that are truly compatible with PBC, the compatibility requirement can be somewhat relaxed in practical DD simulations. For example it is possible, starting with a PBC-compatible configuration, to add one or several infinite dislocations that will introduce a small amount of unbalanced dislocation density in the box. Although physically this would introduce a non-zero net lattice curvature that is impossible to accommodate in the infinite translationally-invariant

[1] In a sense, an infinite dipole can be viewed as a loop closed through infinity.

crystal, this curvature can be neglected for as long as $Lb\rho << 1$, where ρ is the density of geometrically-necessary dislocations (GND) added to the box and L is the box size. For a typical box size of 10 μ and the GND density $\rho = 10^{12}$ m^{-2}, the dimensionless ratio above is of the order of 10^{-3}. Whichever initial arrangement of lines is considered, the use of PBC will ensure that Nye's tensor integrated over the box volume is conserved in the course of DD simulations.

Treatment of image stress

Fully consistent application of PBC requires that additional stress associated with the periodic images of dislocation be accounted for. This is the most involved part of the whole implementation. In DD, the lion's share of computations goes to calculations of elastic interactions between dislocation segments. The unit element of such calculations is the evaluation of stress produced at a given material point P by a dislocation segment centered at position S. Using the analytical formulae developed in the continuum theory [3, 13], such a calculation takes a few hundred arithmetic operations to obtain all six components of stress from a general dislocation segment of finite length. In PBC, the computational burden increases many-fold because stress from the periodic images of the primary segment has to be evaluated. Considering that the overall effort already scales as $O(N^2)$, where N is the number of dislocation segments, the brute force treatment of image stress in PBC becomes prohibitive. Earlier, one of us found a practical solution in a similar situation, for computationally expedient evaluation of periodic corrections to the elastic Green's function in 2D [14]. The idea was to pre-tabulate the correction stress on a regular grid within the computational volume and then use these grid values for fast interpolation. The interpolation itself is based on the minimum image convention which dictates that the total stress due to a given segment and all of its periodic images, is associated with the replica of the segment that is nearest to the field point (Fig. 2). Practically, the calculation requires that the box is centered on the field point, and the look-up procedure goes over all segments, primary or replicas, that fall inside this box.

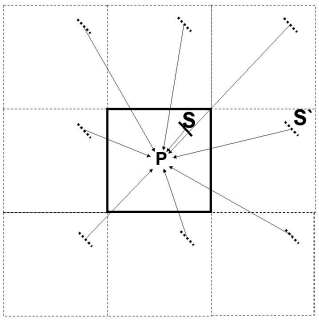

Fig. 2 *Periodic lattice of image*

Extension of this idea to DD simulations in 3D encounters considerable but manageable difficulties. The most obvious of them is the high dimensionality of the required look-up tables. To improve the situation we created the tables only for differential, or point-like dislocation segments, i.e. such segments whose length is considerably smaller than their distance to the field point. Compared to the case of straight segments of finite length, the use of point-like segments reduces the dimensionality of the tables from four to three. Still, it appears one needs to pre-calculate 54 image correction tables, one for each of the six components of stress generated by nine components of the tensorial charge $dl\mathbf{b} \otimes \mathbf{t}$ (here dl is the length of the differential segment). However, using cubic periodic boxes and taking advantage of the cubic symmetry, the number of independent tables can be reduced from 54 to eight. The same symmetry allows reduction of the amount of computations by 48 times, by considering only the grid points in the irreducible zone of the cube. This also reduces the amount of memory required to store the tables, if this is a limiting factor. For a given accuracy of interpolation, the number of grid points

can be reduced by making the tabulated functions as smooth as possible inside the cube. Since the stress field of the nearest image of the segment diverges as $1/r^2$ at the origin, we exclude the nearest image from the correction tables and evaluate its contribution analytically instead. This eliminates the singularity since all the replicas other than minimum images lie outside the box by definition.

The most serious problem we had to face was *conditional convergence* of the lattice (Madelung) sums that need to be evaluated for every entry of the stress correction tables. In a forthcoming publication we present a thorough discussion of this important mathematical aspect of the continuum theory of dislocations. Here we only briefly recount that the naïve lattice summation of the stress terms associated with the primary and replica segments is convergent, but the end result depends on the order of summation. In general, such conditional sum gives rise to an arbitrary average stress in the simulation cell which will cause problems for DD simulations. The physically meaningful part of the Madelung sum is therefore the stress field variation over the simulation cell, which converges absolutely and thus does not depend on the order of summation. We have implemented an effective numerical procedure *MadSum* for subtracting the spurious parts of the lattice sums and used the remaining stress field variations as the entries for the stress correction tables.

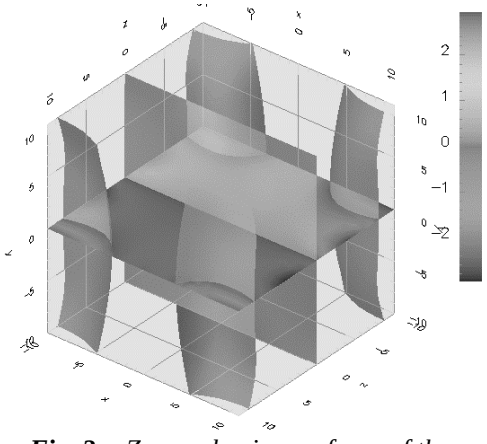

Fig. 3. *Zero-value iso-surfaces of the tabulated stress correction term for σ_{13}, interpolated in the unit cube as a function of segment position. Note zero-value region near the origin.*

Fig. 3 is an example of one such correction function tabulated on a cubic grid 32 x 32 x 32 in the unit cube. Several features of this function are noteworthy. First, the displayed function retains periodicity and some symmetries of the cube. Second, except for several symmetry lines, the function is non-zero on the cube faces. This observation calls in question the use of a cut-off distance for reducing the cost of computing the interactions between dislocation segments in DD simulations in 3D. Third, the correction function is zero in the center of the cube, indicating that within some radius (~0.2 of the cube size) no correction is needed. In the context of large-scale DD simulations, elastic interactions between the segments beyond certain range are usually evaluated using the multipole expansion techniques. That the correction functions are zero around the cube center, suggests a procedure in which only the multipole terms are corrected, whereas interactions between the segments at a shorter range require no correction at all. Comparison of the computational cost among the different ways of treating the interaction stress reveals that numerical interpolation of the image-corrected stress takes some four times longer than the analytical evaluation of stress from the same number of dislocation segments. However, because the number of multipole momenta that have to be corrected is generally smaller than the number of segments demanding "personal attention", the total amount of time spent on analytical (uncorrected) and numerical (image-corrected) stress evaluation, are comparable.

SUMMARY

In this short contribution we intended to show that there is nothing particularly nasty about PBC as the boundary conditions for DD simulations in 3D. On the other hand, with the obvious advantage of retaining translational invariance and effectively eliminating the boundaries, PBC are well positioned for 3D simulations of single crystal plasticity in the bulk. As always, one has to be vigilant and watch for the artifacts associated with the small system size. In particular, any length scale emerging in the simulations that appears comparable to the periodic box size, should be treated with suspicion. Interaction of dislocations with their own images may be a cause of spurious effects, e.g. artificially enhanced dislocation recombination or formation of strong dipoles immobilizing the dislocations. In particular, the use of cubic boxes for the high symmetry FCC and BCC systems will cause each slip plane to self-connect after two periodic translations. Although various fixes to alleviate such undesirable behaviors can be devised, in our view there is only one real solution. It is to make the system large enough so that the finite size effects become insignificant. For example, to avoid spurious reconnection before one percent of plastic strain is accumulated (assuming dislocation density $\rho = 10^{12}$ m^{-2}) the cube should be at least 20 μ on the side. Obviously, periodic boundary conditions do not make the system infinite. Nonetheless, they hold considerable computational advantages over the other types of boundary conditions currently employed for 3D simulations of bulk crystal plasticity.

ACKNOWLEDGEMENTS

We thank T. Diaz de la Rubia, N. Ghoniem, H. Huang, D. Lassila, K. Schwarz and L. Wickham for their continued interest and support. This work was performed under the auspices of the U.S. DOE by LLNL under contract No. W-7405-ENG-48. WC acknowledges support from LLNL under an ASCI-level 2 award. VVB and MR acknowledge support from the Office of Basic Energy Sciences, the U.S. Department of Energy.

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