Periodic Boundary Conditions for Three Dimensional Dislocation Dynamics

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Periodic Boundary Conditions for Three Dimensional Dislocation Dynamics

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ABSTRACT

The boundary conditions in three dimensional Dislocation Dynamics (DD) simulations have always been a matter of concern. Two types of boundary conditions, quasi-free-surface and reflection boundaries are currently being used by groups in Grenoble, France and Pullman, Washington. In this paper, we present a mathematical transformation that enables simulations of dislocation evolution processes in single crystals using periodic boundary conditions (PBCs). The idea is graphically demonstrated with transformation matrices given for BCC crystal systems. Extension to other crystal structures is also discussed. Comparing to the existing boundary conditions, the new approach (1) balances the dislocation flux in and out of a computational cell; and (2) does not require artificial termination of dislocations in the bulk.
1. Introduction

PBCs have been used in two dimensional DD simulations (e.g., [1]), because slip planes can be chosen so that their normal vectors lie parallel to the two axes. The PBCs therefore bring a dislocation segment leaving the computation cell back to the same slip plane. In three dimensional DD simulations, however, this cannot be readily accomplished in a straightforward manner. At present, quasi-free-surface [2] and reflection [3] boundary conditions are being used. However, these boundary conditions introduce some undesirable artificial constraints into bulk simulations. In this note, we propose a new approach that enables the use of PBCs in three dimensional DD simulations.

There are 4 and 18 slip planes for the FCC and the BCC crystal systems, respectively (assuming {110} and {112} slip planes only for BCC), and it is impossible to make the normal vectors of all slip planes parallel to the axes of a three dimensional coordinate system. Therefore, PBCs cannot always bring a dislocation segment back to the same slip plane when it glides across the computational cell boundary. Taking the BCC crystal system as an example, this problem is demonstrated in Figure 1. Only one slip plane, the normal vector of which is not parallel to any axis, is shown for clarity. In single crystal DD simulations, only segments of dislocations are included in the computational cell. To make these segments move as if they were in a bulk, they must interact with segments outside of the computational cell. When a segment, e.g., AB in Figure 1, glides it must stay on the same slip plane. If a PBC is applied to the coordinate system in Figure 1, B will be connected to B’ which is on a different slip plane. This introduces unphysical cross slip and therefore erroneous dislocation structures.

In this paper, we present a mathematical method that makes the normal vector of every slip plane parallel to an axis of the coordinate system employed in the three dimensional DD simulations. Instead of using a single coordinate system, we place dislocations on various coordinate systems according to their slip systems (slip planes and the Burgers vectors). In each coordinate system, there are two slip planes and their normal vectors are parallel to two axes of the coordinate system. In Section 2, the idea is demonstrated graphically with transformation matrices formulated for the BCC crystal systems. The idea is summarized in Section 3. Applications of this idea to other crystal systems are also discussed in the final Section.

2. Periodic Boundary Conditions
terminating dislocations in the bulk of a solid, we have to represent a dislocation segment by AB, i.e., A and B have to be connected. This constraint can cause artificial dislocation clustering if the computational cell is too small such that a dislocation segment interact strongly with its own image across the periodic boundary. However, the constraint is not severe anymore as the computational cell is large enough. For a computation cell of 10 micron in linear dimension, interaction of a dislocation segment with its own image across the periodic boundary is less than 1% of that with its neighbors (assuming dislocation spacing to be <100nm). Comparing to any of the existing boundary conditions, this new approach have the following two advantages: (1) it balances flux in and out of the computational cell automatically; and (2) dislocations are not terminated in the bulk of a solid.

3. Summary and Discussion

Using a mathematical method, we have developed a scheme which enables application of PBCs in three dimensional DD simulations. The model can be summarized as follows:

(1) Dislocations are partitioned among twelve coordinate systems in the BCC crystal system. Each coordinate system can be periodically repeated satisfying: (a) flux balance and (b) no-termination of dislocations in the bulk.

(2) A dislocation segment in one coordinate system interacts with dislocations in all coordinate system. It can also move to other coordinate systems via cross slip.

(3) Even though only {110} and {112} planes are considered as slip planes, the method can be easily extended when {123} or other slip planes are included as well by adding several more coordinate systems.

(4) The method, demonstrated for the BCC structure is applicable to all other crystal systems. For example, an FCC crystal system has {111} slip planes and <110> Burgers vectors. With a <111> and a <110> as two axes, the third axis can be chosen as a <112> so that an orthogonal coordinate system is obtained. The number of coordinate systems depends on specific crystal structures.

Acknowledgment

Discussions with George Gilmer at Bell Labs, Nasr Ghoniem at UCLA, Moono Rhee, Hussein Zbib, and John Hirth at WSU are greatly acknowledged.
Instead of placing all dislocations on one coordinate system, we partition the dislocations among twelve coordinate systems according to their slip systems. In each coordinate system, two axes are defined as normal vectors of slip planes, while the third axis is the Burgers vector. One of the coordinate system is shown in Figure 2, where normal vectors of two slip planes, [110] and [112], and the corresponding Burgers vector, [111], constitute an orthogonal coordinate system. With PBCs, a dislocation segment AB leaving the right boundary is brought back to the computation cell at B' which coincides with A. Infinitely repeating this computational cell will map the whole space. First, the dislocation going through a periodic boundary stays on the same slip plane. Secondly, the dislocation does not have to terminate in the computational cell, which is a necessary condition when an inner section of a single crystal is studied. Axes of all the twelve coordinate systems are listed in Table 1. The first column is the assigned identification number to each coordinate system. Columns 2 to 4 are the three axes in each coordinate system. A dislocation segment in one coordinate system interacts with dislocations in all coordinate system. A dislocation segment can also move from one coordinate system to another, corresponding to cross slip. A dislocation can cross slip only when it is pure screw and has the same Burgers vector on the two slip planes. Therefore, a dislocation segment can move from one coordinate system to another only when the two coordinate system share the same X axis (parallel or anti-parallel to the Burgers vector). When interaction of two dislocation segments in two different coordinate systems is concerned, dislocation coordinates must be transformed between the coordinate systems. A point in a three dimensional space (or simply a vector) can be represented as:
\[
\mathbf{r} = x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3
\]
\[
= x'\mathbf{e}_1' + y'\mathbf{e}_2' + z'\mathbf{e}_3'
\]
where \((\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)\) and \((\mathbf{e}_1', \mathbf{e}_2', \mathbf{e}_3')\) are normalized unit vectors of any two sets of orthogonal coordinate systems. The coordinates are related by the following equation:
\[
\begin{bmatrix}
  x' \\
  y' \\
  z'
\end{bmatrix}
= \begin{bmatrix}
  \mathbf{e}_1 \cdot \mathbf{e}_1' & \mathbf{e}_1 \cdot \mathbf{e}_2' & \mathbf{e}_1 \cdot \mathbf{e}_3' \\
  \mathbf{e}_2 \cdot \mathbf{e}_1' & \mathbf{e}_2 \cdot \mathbf{e}_2' & \mathbf{e}_2 \cdot \mathbf{e}_3' \\
  \mathbf{e}_3 \cdot \mathbf{e}_1' & \mathbf{e}_3 \cdot \mathbf{e}_2' & \mathbf{e}_3 \cdot \mathbf{e}_3'
\end{bmatrix}
\begin{bmatrix}
  x \\
  y \\
  z
\end{bmatrix}
\]
(2)
All the twelve coordinate systems listed in Table 1 are orthogonal, and coordinates among them are therefore related by equation (2).

However, a restriction has been placed on the dislocation segment. If the dislocation segment is AC instead of AB, the PBC will bring C to C' which is not the same as A. In this case, a dislocation is unphysically terminated inside a single crystal. To avoid
References:

Figure Caption:

Figure 1: A dislocation on a (110) slip plane, the normal vector of which is non-parallel to any of the axes.

Figure 2: A dislocation in one of the twelve coordinate systems.
Table 1: Coordinate systems

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Fig 1
Fig 2