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A novel approach to study dislocation density tensors and lattice rotation patterns in atomistic simulations

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ABSTRACT

Crystal plasticity caused by the nucleation and interaction of dislocations is an important aspect in crystal deformation. Recent nanoindentation experiments in single crystals of copper or aluminum revealed large deviations in the lattice rotation and an inhomogeneous distribution of the dislocation density in the plastic zone under the indenter tip. Molecular dynamics simulations offer the possibility to study the origin of these phenomena on an atomistic scale, but require sophisticated analysis routines in order to deal with the massive amount of generated data. Here a new efficient approach to analyze atomistic data *on the fly* during the simulation is introduced. This approach allows us to identify the dislocation network including Burgers vectors on the timescale of picoseconds and below. This data does not only reveal the evolution of dislocation structures, but it offers the possibility to quantify local dislocation density tensors calculated on an atomic level. The numerical results are compared with experimental data from the literature. The presented approach provides useful insight into the active deformation mechanisms during plastic deformation that will help us to bridge simulations on atomic scales and continuum descriptions.

1. Introduction

The distribution of lattice rotations and geometrically necessary dislocations (GNDs) under an indenter tip during nanoindentation has recently attracted attention in both experiments (Zaafarani et al., 2006, 2008; Kysar et al., 2007; Larson et al., 2007; McLaughlin and Clegg, 2008; Demir et al., 2009) and simulations (Zaafarani et al., 2006, 2008; Demir et al., 2009; Bouvier and Needleman, 2006; Hua and Hartmaier, 2010). Cross-sectional cuts through the indented material show patterns of rotations and counter-rotations, as well as an inhomogeneous distribution of GNDs in face centered cubic (FCC) metals. Although experimental results are a valuable source of information, high resolution observations are only available *post-mortem* and can therefore not capture the ongoing mechanisms of plasticity on very small scales; a gap that can be bridged by simulations. In the present work we study the lattice rotation patterns and dislocation densities during nanoindentation in copper single crystals on an atomistic scale using molecular dynamics (MD). In contrast to classical continuum mechanics simulations, MD does not rely on a model for material response. Instead the response in MD is a result of atomic interactions, making it a powerful tool to gain insight into material behavior at small scales, where dislocations are the most important lattice defect during plastic deformation.

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Because of the extremely large number of dislocations even in a well annealed crystal, only densities of dislocations are used to characterize the dislocation microstructure in experiments on the microscale. On the nanoscale two definitions of dislocation densities are feasible and will be used to analyze the performed simulations. The density of dislocations can be either defined as a scalar value, computed by dividing the total length of all contained dislocations by a reference volume v, or as a dislocation density tensor (DDT)

$$\alpha = \frac{1}{v} \oint_{\perp \text{ in } v} d\underline{l} \otimes \underline{b}, \tag{1}$$

where the line direction $\underline{l}$ and the Burgers vector $\underline{b}$ of each dislocation is taken into account. The GND is considered to be the minimum amount of dislocations in a finite volume to preserve the continuity of a lattice in the presence of strain gradients and is related to the DDT. As opposed to a scalar dislocation density, the DDT does not consider dislocations of opposite Burgers vectors within the same volume element. Such dislocations, called statistically stored dislocations (SSDs), neither produce strain gradients nor do they contribute to the lattice rotation (Gao et al., 1999).

The DDT α, also called the Nye-tensor, is directly related to the lattice curvature K as presented in the work of Nye (1953), by

$$K = 1/2(\text{tr } \alpha)I - \alpha^T, \tag{2}$$

where I denotes the identity matrix. Therefore, by measuring the local curvature within a crystal, it is possible to derive the DDT. This approach to obtain local GND densities has been applied in experimental studies using X-ray microscopy by Larson et al. (2007) or in electron backscatter diffraction (EBSD) tomography by Demir et al. (2009).

By calculating the local curvature caused by lattice rotations on the atomistic scale, GNDs can be derived from atomistic data in a similar approach to experiments. A far more precise alternative is however the application of Eq. (1), but this approach requires the knowledge of the dislocation network. The task of obtaining dislocation networks from large scale atomistic simulations of plasticity, consisting of millions of atoms, is highly non-trivial. Neither is *a priori* information concerning dislocations and their Burgers vectors available, nor are there explicit dislocation entities present. The dislocation network has to be extracted purely from atomic coordinates. Recently Stukowski and Albe (2010a,b) published two methods to acquire this kind of data, where Burgers vectors are identified by constructing minimal Burgers circuits around defect structures. Here we present another solution for this task, in which the Nye-tensor analysis method as described by Hartley and Mishin (2005a,b) is extended and integrated into the method of dislocation line extraction (Begau et al., 2011). Combining both methods enables a fully automated process to obtain dislocation networks including Burgers vectors and to derive dislocation densities and dislocation density tensors.

2. Methods

2.1. Obtaining Burgers vectors from dislocation density tensors

This section introduces the modifications to the original Nye-tensor method, an approach to derive Burgers vectors without constructing Burgers circuits explicitly, and its coupling with the dislocation line extraction (skeletonization) method, to identify dislocation networks. For details concerning the implementation of the original Nye-tensor method we refer to the work of Hartley and Mishin (2005a,b).

The definition of an atomistic scale dislocation density tensor α is fundamental to compute Burgers vectors in this approach. We use the form

$$\alpha = -(\nabla \times G), \tag{3}$$

where G denotes the local deformation tensor, that characterizes the elastic distortion in the vicinity of an atom by mapping the current lattice configuration $d\underline{x}'$ back to a perfect reference lattice configuration $d\underline{x}$, i.e.

$$d\underline{x} = d\underline{x}' \cdot G. \tag{4}$$

The affine transformation G is calculated numerically per atom by finding the least square solution between the set of nearest neighbor bonds in the deformed and the bonds in the reference crystal. The mapping between both sets of bonds is found by comparing their angular deviation. Hartley and Mishin (2005a) suggest to ignore bonds, for which no corresponding bond with an angle of less than 27° in a perfect crystal is found. However, with the modifications presented here a smaller threshold of 20° yields more satisfying results.

In the following section it is necessary to distinguish between two different kinds of Burgers vectors, the resultant Burgers vector (RBV) and the true Burgers vector (TBV). The RBV is a value numerically computed per atom, where the TBV denotes a crystallographic correct Burgers vector of a dislocation. At first the method to obtain RBV is introduced, and then it is shown how these values are mapped to TBVs.

The relation between the Burgers vector $\underline{b}$ and the dislocation density tensor α is

$$\underline{b} = -\int_A (\alpha \cdot \underline{l})\, ds, \tag{5}$$

where A denotes a surface enclosing the distribution of α around a dislocation core and $\underline{l}$ the dislocation line direction. Therefore, a numerical integration of α provides the resultant Burgers vector, assuming the dislocation line direction is known.