Development of a method to determine Burgers vectors from atomistic data

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Abstract. Large-scale molecular dynamics simulations have been widely used to investigate the mechanical behaviour of materials. But complex datasets, involving the positions of millions of atoms, generated during the simulations make quantitative data analysis quite a challenge. This paper presents a novel method to determine not only dislocations in the crystal, but also to quantify their Burgers vectors. This is achieved by combining geometrical methods to determine the atoms lying in the dislocations cores, like for example the common neighbour analysis or the bond angle analysis, with the slip vector analysis. The first methods are used to filter out the atoms lying in undisturbed regions of the crystal; the latter method yields the relative slip of the remaining atoms and thus indicates the Burgers vector of those atoms lying in the dislocation cores. The validity of the method is demonstrated here on a single edge dislocation in a relatively small sample. Furthermore a way will be sketched how this analysis can be used to determine densities of statistically stored and geometrically necessary dislocations, respectively. Hence, this method can be expected to provide valuable input for strain gradient plasticity models.

1. Introduction

Atomic scale computer simulation such as Molecular Dynamics (MD) is a powerful tool for revealing the processes underlying the plastic response of a crystal and for providing valuable insights into its material behavior. The important goals of atomistic studies of confined geometries, like nanoindentation, are to identify the atomistic mechanisms in the early states of plastic deformation under the indenter, to characterize the defect structures and even to directly compare force-indentation behaviour with experiments.

The analysis of atomic bonds is widely used in large-scale molecular dynamics simulations to characterize the state of a local crystal structure. Most local structure analysis methods such as the centrosymmetry parameter (CSP) [1] and the common neighbor analysis (CNA) [2] use such abstractions to characterize the local state of solid materials. Ackland and Jones [3] take advantage of the bond angular distribution (BAD) function to distinguish the crystal types of body centered cubic (bcc), face centered cubic (fcc) and hexagonal close packed (hcp). This BAD analysis is faster and gives fewer false positive results (atom lying in a defect is identified as bulk atom) and negative results (bulk atom identified as defect atom) than previous methods. The slip vector analysis (SVA), developed by Zimmerman et al [4], compares the current atomic configuration to a reference state and thus quantifies the local atomic slip in the ensemble. The slip vector is a measure of local plastic
deformation and is related to the Burgers vectors of a lattice dislocation that caused this plastic slip. This method has been shown to be capable of detecting different contributions to plastic slip from atomistic simulations [5].

In our approach, we combine SVA and BAD to yield the magnitudes and directions of plastic slip of atoms situated in dislocation cores. The objective of our research work is to provide an atomic level insight into plastic deformation mechanisms during nanoindentation and utilize all the information of the atomic data to make the calculation of signed dislocation densities and dislocation density tensors possible.

2. Burgers Vector Analysis

The slip vector developed by Zimmerman [4] is defined as

\[ \mathbf{s}^{(k)} = -\frac{1}{n_s} \sum_{l=1}^{n_s} (\mathbf{x}^{(kl)} - \mathbf{X}^{(kl)}) \]

where atom \( l \) is a nearest neighbor of atom \( k \), \( n_s \) is the number of the slipped neighbors, \( \mathbf{x}^{(kl)} \) and \( \mathbf{X}^{(kl)} \) are the position vector difference between atom \( k \) and \( l \) in the current and reference configurations, respectively. The reference configuration denotes the arrangement of atomic positions at the beginning of the deformation step.

The slip vector is a measure of the local plastic deformation since it denotes the average displacement of an atom in its current position compared to the initial position and relative to its nearest neighbors. However, the slip vectors of atoms lying on opposite sides of the slip plane point in opposite directions. Hence, we have to develop a way to uniquely define the direction of the slip vector, before we can associate it with plastic slip in the crystal. To accomplish this, we identify the atoms situated in dislocation cores with the help of the bond angle analysis method [3] and only analyze the slip vector within the dislocation core. Furthermore, by identifying those atoms with a higher coordination number than bulk atoms, we can identify the atoms in the core of an edge dislocation that lie on the side of the slip plane where it intersects the inserted half-plane. In fcc crystals, we typically find atoms with coordination numbers of 13 on this side of the slip plane. On the opposite side of the slip plane, in contrast, we find atoms with a smaller coordination number than bulk atoms. By using this property of edge dislocations that allows us to define an “upper” and “lower” side of the slip plane, we are able to define a unique direction of the plastic slip that is characterized by the slip vector of atoms in the dislocation core.

To demonstrate the method, a copper crystal (97,296 atoms) containing a single edge dislocation as shown in figure 1 is studied here. The size of the crystal prior to deformation is 40x6x17 unit cells which correspond to a volume of 202.8x53.0x106.4 Å³. For simplicity, and since we only want to demonstrate the analysis method, we use rather simple geometry, where the top surface is a crystallographic (111) plane with free boundary conditions, the bottom surface is fixed, and periodic boundary conditions are applied to the sides of the simulation box. The simulations using an embedded atom method (EAM) potential for Cu developed by Mishin et al. [6] are conducted in the NVE (constant number of atoms, constant volume, constant energy) ensemble. The MD simulations were performed using a version of the IMD parallel molecular dynamics code [7] in which we implemented the BAD and SVA methods. For visualization, the atomistic configuration viewer Atomeye [8] and the Tecplot software were used.

Before mechanically loading the simulation box, the dislocation has been properly relaxed, until all atoms found the energetic minimum position, which corresponds to a simulation at \( T=0 \)K. As it is well-known, a perfect edge dislocation in the fcc structure is dissociated into a leading and a trailing Shockley partial gliding on the (111) slip plane and linked by a stacking fault. Here, the dissociation reaction for copper is given by:
The lattice constant of copper is \( a = 3.615 \text{ Å} \). The Burgers vector magnitude of copper is \( b_{\text{partial}} = 1.48 \text{ Å} \) for a \( \{111\}<112> \) partial dislocation and \( b_0 = 2.56 \text{ Å} \) for a perfect \( \{111\}<110> \) dislocation.

Finally the relaxed ensemble is loaded with a shear stress of 300 MPa in a dynamic simulation with a time step of 0.001 ps for 90 iteration steps. During this simulation, the edge dislocation glides on the \( \{111\} \) plane under the action of the applied shear stress. Figure 1(a) shows the atomistic configuration of the lower half of the simulation box. In figure 1(b) the result of the slip vector analysis for the atoms lying below and above the slip plane are shown, while in figure 1(c) only the slip vector of the atoms lying in the dislocation core is represented, by combining the BAD and the SVA method. Furthermore, in this figure the sign of the slip vectors lying above the slip plane have been flipped, such that all vectors point in the same direction. The vectors shown in figure 1(c) thus represent the Burgers vector of the dislocation on the atomic scale.

In figure 1(b), there are four groups of atoms represented by the slip vectors: (i) atoms lying in the wake of the dislocation with a full Burgers vector as slip vector (dark blue), (ii) atoms in the stacking fault region with a partial Burgers vector as slip vector (light blue), (iii) atoms in the leading partial dislocation core, and (iv) atoms in the trailing partial dislocation core (green, red, and orange). Since in each group the slip vector is almost the same, here we only choose one atom of a group to analyze. A closer analysis shows that the atoms in the stacking fault region have slip vectors of \((-1.19, 0.61, 0.58)\) in the crystallographic orientations of \([110]\), \([\overline{1} \overline{2} 2]\) and \([111]\). The magnitude of this slip vector is 1.46 Å which is very close to the magnitude of the partial Burgers vector \(b_{\text{partial}}\). The direction of this slip vector is close to \((-1.0, 0.5, 0.5)\) which is actually the leading Shockley partials of \([\overline{2} 11]\). So in fact, this part can be identified as Burgers vector of the leading Shockley partial dislocation. The slip vectors of atoms in the dislocation core are not in such good agreement with the expected full Burgers vectors. This is seen by the analysis of an atom in the trailing partial core, which has the slip vector components \((-1.41, 1.19, 0.32)\). The direction of this slip vector is reasonably close to the \((-1.0, 1.0, 0)\) vector, i.e., the complete Burgers vector. The magnitude of this slip vector is 1.87 Å and thus smaller than \(b_0\), which shows the lattice slip is still incomplete in the dislocation core.
Figure 1. The atomistic configuration of an edge dislocation and the corresponding Burgers vector analysis. In figure 1(a) a cut through the atomistic configuration is shown, where the atoms are color coded according to the BAD analysis (dark red: surface, dark blue: fcc, light blue: stacking fault (hcp), green: 12 neighbors, neither fcc, nor hcp, orange: 11 neighbors); Figure 1(b) shows the results of the slip vector analysis for the atoms lying in the slip plane of the dislocation; in figure 1(c) only the slip vectors of the atoms lying in the dislocation core are shown, and the sign of the slip vectors of the atoms on top of the slip plane have been flipped. All slip vectors are normalized with the norm of the Burgers vector $b_0$.

3. Summary and Outlook

Through the above analysis, we have successfully identified Burgers vectors purely from atomistic data of a sample containing an edge dislocation in fcc copper. This is accomplished by combining the slip vector analysis and the bond angle distribution method. The method has already been tested for more complex situations, as for example the dislocation structure underneath a nanoindenter in fcc copper and also in bcc tungsten. These results will be published in forthcoming work. This method, hence, opens the way to calculate signed dislocation densities and dislocation density tensors directly from atomistic data. The knowledge of the dislocation density tensor, in turn, allows plastic strains and work hardening to be calculated for each slip system independently. Thus, the condensed information gained on the atomic scale can be incorporated into continuum mechanics methods through Orowan law or Taylor work hardening rules in a multiscale modeling approach.

References

[1] Kelchner C L, Plimpton S J and Hamilton J C 1998 Phys. Rev. B 58, 11085
[2] Honeycutt J D and Andersen H C 1987 J. Phys. Chem. 91 4950
[3] Ackland G J and Jones A P 2006 Phys. Rev. B 73 054104
[4] Zimmerman J A, Kelchner C L, Klein P A, Hamilton J C and Foiles S M 2001 Phys. Rev. Lett. 87 165507
[5] Vo N Q, Averback R S, Bellon P, Odunuga S and Caro A 2008 Phys. Rev. B 77 134108
[6] Mishin Y, Mehl M J, Papaconstantopoulos D A, Voter A F and Kress J D 2001 Phys. Rev. B 63, 224106
[7] http://www.itap.physik.uni-stuttgart.de/~imd/userguide/imd.html, University of Stuttgart, Institute of Theoretical and Applied Physics (ITAP).
[8] Li J 2003 Modelling Simul. Mater. Sci. Eng. 11, 173