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A topologically correct method of dislocations construction for atomistic modeling

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ABSTRACT

We discuss the deep topological reasons why dislocation quadrupoles should be used for the construction of dislocations containing edge components. We demonstrate that contrary to all other currently used methods, this approach exactly preserves the topology of the order parameter field (atomic displacements in a crystal with defects relative to a defect-free crystal) of a dislocation-free crystal with periodic boundary conditions even for small simulation volumes and, thus, restores the verity of the material frame indifference principle, broken in other techniques. Using dislocation quadrupoles for edge and mixed dislocations, we have developed a careful procedure for relaxation of atomic positions around a dislocation core which enables one to achieve arbitrary low dislocation densities characteristic for real crystals. As a demonstration of the method capabilities, we have constructed a simulation volume with as low dislocation density as $1.5 \cdot 10^{14}$ m^{-2}, which is realistic in deformed crystals, and one can easily lower this value as desired. All details of dislocation construction process are explicitly specified, making it very easy to reproduce our results. FCC Al crystal is used as a test case.

1. Introduction

Since the realization of the crucial role dislocations play in metals plasticity [1], a lot of efforts, both experimental and theoretical, have been spent in attempts to understand the physical mechanisms underlying the phenomenon and its dependencies on stress, strain rate, and temperature [2]. Qualitative predictive description of the plastic deformation process is an extremely complex task as it is influenced by the physical phenomena proceeding at very different time and length scales — starting from nanometers and fractions of nanosecond up to macroscopic lengths and years (in the case of plastic deformation with slow strain rate — creep). This is partially due to the fact that mechanisms of plasticity include not only the motion of dislocations, but an interaction of dislocations with point defects, such as vacancies and interstitials, and obstacles — voids, precipitates, other dislocations, as well. Thus, to understand the nature of plasticity, one has to bridge the gap between microscopic and macroscopic scales, and for this purpose, models of dislocation motion and their interactions with point defects for different scales should be developed.

Various methods are used for dislocation modeling. They basically fall into the three categories. The simplest and the first to appear were continuous mechanics methods based on long-range force fields created by dislocations [1] and the Peach-Koehler expression for the forces acting on dislocations. This method though fast, efficient and viable at the macro scale, is only applicable outside of the dislocation cores, thus the atomic structure of a dislocation core is overlooked. At the same time, as it has been demonstrated in [3], an atomic structure of a dislocation core has a significant influence on dislocation mobility.

On the other pole of the scale lengths hierarchy are fully first-principles quantum-mechanical methods accounting precisely for the atomic positions around a dislocation core. Those methods are highly precise but, unfortunately, limited to the number of atoms of about 1000, which is not sufficient for the investigation of dislocations motion and can be used for the elucidation of the basic properties of dislocation cores. There exist hybrid methods utilizing continuous approaches, like Peierls-Nabarro, parameterized with the results of first-principles calculations of γ-surfaces [4]. They still lack the atomic resolution necessary for obtaining quantitative results.

Perhaps the optimal trade-off between the precision and efficiency of calculations in the area of dislocations modeling is provided by the approaches based on molecular dynamics (MD). Using modern parallel clusters it is feasible to model not only microscopic systems but also mesoscopic, when the number of atoms may reach 10^9 and the simulation times — tens of nanoseconds. Embedded Atom Model (EAM) interatomic potentials employed for metallic [5] systems give quantitative values of equilibrium lattice constants, elastic moduli and

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phonon spectra, comparable to those obtained with quantum-mechanical first-principles approaches. Molecular dynamics results can be further used for parameterization of Discrete Dislocation Dynamics (DDD) methods, allowing for even larger simulation volumes with the linear sizes up to tens of μm. Thus, a simple and efficient method for the construction of an initial dislocation in a simulation volume is vital for the modeling of dislocations motion and their interaction with point defects.

In the process of dislocation construction, one should provide for the following basic conditions to be satisfied. First, there are situations when dislocations should not be placed too densely in a simulation volume, as their mutual influence, due to the long range-force fields produced by them, will distort the external stress applied to a simulation volume. Second, any residual stresses remaining after a dislocation has been constructed should be relaxed, as such stresses can distort the picture of dislocation motion. Note that a Peierls stress in FCC metals can as low as $10^{-5}G$, where G is a shear modulus [2]. This second requirement is especially important if a simulation volume is of moderate size which can be the case, for example, when one is interested in the modeling of dislocations pile-up at grain boundaries. And finally, since periodic boundary conditions are very popular in molecular dynamics calculations, an algorithm of dislocations construction should provide for the correct topology of the order parameter field (atomic displacements in a crystal with defects relative to a defect-free crystal), when periodic images are attached.

There are two approaches to the construction of dislocations described in the literature. The earlier methods such as Rigid boundary model (RBC) and Green's function boundary conditions (GFBCs) [6] have serious limitations such as difficulty to achieve the motion of dislocations or computational inefficiency due to the calculations of long-ranged Green's functions. The modern techniques usually use periodic arrays of dislocations (PAD) [5].

Specific details of how PAD is realized may vary. In the first approach [7–9], the two halves of a simulation volume contain the quantities of atomic planes differing by 1. After the relaxation, the unstrained simulation volume has a wedge shape, and after making it rectangular, residual stresses, different in the upper and lower parts of the simulation volume, appear.

In another approach parts of atomic planes perpendicular to both the Burgers vector and the glide plane are removed from a crystal with the subsequent relaxation of atomic positions [10–12]. In [10,11] dislocation dipoles are created, but the dislocations of opposite signs are located strictly one above another, in the same plane. This results in the number of atomic planes perpendicular to the Burgers vector being different for various heights above and below the glide plane and may lead to residual stresses in this direction, preventing construction of the simulations volume periodic images. In [12] the two atomic half-planes removed from the simulation volume are separated in the direction along the Burgers vector, and the initial gap for the second dislocation starts right where the gap for the first dislocation ends in the direction perpendicular to the glide plane. But for some reason, the authors of [12] refused to use periodic boundary conditions in the direction perpendicular to the glide plane and introduced 5 Å gaps above and below the simulation volume.

Besides the possible residual stresses, another serious problem encountered in the process of dislocations construction is the difficulty in achieving realistic dislocation density. This is partially related to the limitations of the computational hardware and partially to the fact that optimization of a function of several hundred thousand or even million variables (atomic positions), necessary for the construction of a potential energy local minimum corresponding to a dislocation, is a very hard task. The minimal dislocation densities obtained using current methods of dislocations construction are rather high, and can be only found in heavily deformed crystals. The values of dislocation density (where they are specified, or can be deduced from the simulation box dimensions) are $2{\cdot}10^{16}\,\mathrm{m}^{-2}$ in [10], $2.2{\cdot}10^{15}\,\mathrm{m}^{-2}$ in [12] and $1.7{\cdot}10^{15}\,\mathrm{m}^{-2}$ in [8]. Moreover, the procedure of relaxation applied to an initial configuration to create dislocation is not described in detail anywhere, whereas as it has been already mentioned, this task is not trivial at all.

But perhaps the greatest deficiency of the majority of the existing methods used for dislocation construction is that they violate the topology of the order parameter field (atomic displacements in a crystal with defects relative to a defect-free crystal) of a dislocation-free crystal not only on the local scale, in the vicinity of dislocations, but on the global scale as well. When using periodic boundary conditions, this topology change will result in the violation of the material frame indifference principle. Thus, when introducing dislocations care should be taken not to break the topology of the dislocation-free crystal order parameter.

To overcome this deficiency, the authors of [13] suggested using dislocation quadrupoles. Surprisingly, this brilliant idea got much less attention than it deserves. Dislocation quadrupoles were used just occasionally for construction of dislocations, and mostly for the screw dislocations, where the above mentioned problems do not appear [14–16]. In this paper, we elucidate the deep topological reasons why using dislocation quadrupole is the preferred method of dislocation construction if a dislocation contains an edge component. As we argue in the current paper, using a single dislocation in a simulation volume or even a dislocation dipole will not suffice for this purpose.

In the majority of research articles on dislocation dynamics simulations, dislocations of pure type — either edge or screw are initially introduced into a simulation volume. In real crystals, dislocations are of the mixed type, possessing both edge and screw components. Therefore some fine details of dislocation dynamics and their interaction with defects, that depend on mutual orientations of Burgers vector and dislocation line may be lost in simulations. Of the recent papers dealing with mixed type dislocations, one can mention [17]. However in [17] the value of dislocation density — $2.4{\cdot}10^{15}\,\mathrm{m}^{-2}$ is rather high, and using dislocation dipole results in breaking the correct topology of the order parameter.

Thus, it would be of high importance to devise an algorithm which would provide an efficient, reliable and easily reproducible method for dislocations construction, capable of addressing all the discussed issues, that at the same time will enable one to obtain dislocation densities characteristic for crystals, not just heavily deformed, but strain-free. Such algorithm has been suggested in the current paper.

2. Method

2.1. Dislocation quadrupole

A dislocation with an edge component is a topological defect since it implies the presence of extra or missing parts of atomic planes [18]. In approaches where a single dislocation or a dislocation dipole is introduced in a simulation volume, the number of planes along a dislocation line (x-direction) and planes parallel to a slip plane (with the normal along the z direction) is invariant relative to the positions in the yz and xy planes respectively. On the contrary, the number of planes in the y direction, perpendicular to the first two axes (in the case of a purely edge dislocation the Burgers vector is aligned along this direction) depends on the position in the xz plane.

If one introduces an order parameter field $\mathbf{u}(\mathbf{r}) = \mathbf{u}^{\mathrm{disl}}(\mathbf{r}) - \mathbf{u}^{0}(\mathbf{r})$ equal to the atomic shifts in a deformed crystal relative to an ideal crystal, and then keeps track of its values while circling around a dislocation with an edge component, due to different numbers of atomic planes passed by the left and right parts of such contour, the magnitude of $u_y(\mathbf{r})$ will not return to its original value u_y^{start} when one returns to the starting point, but instead will acquire some additional Δu_y. This effect is illustrated in the left frame of Fig. 1. As one is moving along the left or right parts of the contour, Δu_y increases, and moving along the top and bottom parts of the contour does not change Δu_y. The z component