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Nucleation and growth of dislocation loops in Cu, Al and Si by a concurrent atomistic-continuum method

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Submicron-sized samples with 42,000 finite elements containing up to ~86 million atoms have been simulated using a concurrent atomistic-continuum method. The simulations reproduce not only nucleation and growth of semicircular dislocation loops in Cu and Al, but also hexagonal shuffle dislocation loops in Si, with the loop radius approaching ~75 nm. Details of leading and trailing partial dislocations connected by intrinsic stacking faults, dislocation loop coalescence through annihilation, and formation of junctions are reproduced.

Keywords: Concurrent atomistic-continuum method; Coarse-graining; Dislocation loop nucleation and growth; Annihilation and junctions

The nucleation and growth of dislocation loops have been extensively investigated by experimental studies in the past half century. It has been observed that dislocation loops nucleate from the interfaces between the precipitates and crystalline matrix at the atomic scale and evolve into large loops with radii of 30–100 nm [1,2], or larger, depending on obstacle/loop spacing. To understand dislocation loop nucleation and growth, numerous molecular dynamics (MD) simulations have been performed [3–5]; dislocation loop radii in MD simulations are typically limited to the order of 10–15 nm as a consequence of the length and time scale limitations of MD. Continuum theory-based simulations, on the other hand, capture development of dislocation loops with large radii but the atomistic features of partial dislocation dissociation and stacking fault formation are excluded [6]. To bridge the domain between several nm and the very large scales at which stacking fault width is small compared to the loop radius, coarse-grained MD or some type of multiscale method is required.

Existing multiscale methods for dislocation-mediated plasticity generally fall into two categories. One approach is hierarchical, such as the discrete dislocation dynamics (DD) method [7–9], wherein dislocations are treated as continuum entities moving through the lattice. A set of constitutive rules, inspired and/or informed by experiments or atomistics, is used to describe the dislocation mobility and interactions of segments. In DD simulations, a curved dislocation line of mixed character is typically approximated using many small linear dislocation segments. Complex dislocation loop interactions may offer considerable challenges for such rule-based descriptions, particularly for loop radii on the order of up to a few hundred nm, since they do not model dissociation. The second multiscale approach is that of concurrent domain decomposition, including the Coupling length scales (CLS) [10] and Quasicontinuum (QC) [11] methods, wherein spatial regions encompassing defects are modeled with full atomistic resolution and other regions by continuum descriptions. However, for example, in regions where dislocations are to be considered, full atomistic resolution is required as QC is not amenable to passing dislocations. This means that the computational cost of QC will increase significantly as the radius of the dislocation loop increases. Another popular concurrent domain decomposition method for dislocation plasticity is the Coupled atomistic and dislocation dynamics (CADD) method developed by Shilkrot et al. [12,13]. Two-dimensional simulations using CADD have shown that this model can capture long-

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range stress fields associated with dislocation pile-ups and can also account for dislocation migration across much larger length scales. To allow dislocations to pass smoothly across the interfaces between atomistic and DD regions, CADD has to be imbued with complex strategies for crossing the interface, which has heretofore limited its application to straight dislocation lines. Passing a dislocation loop through a planar dividing surface would severely tax the strategy. The same difficulty also exists in other multiscale methods, such as the Extended finite element (XFEM) + Bridging domain method (BDM) method [14]. To date, no multiscale method that connects atomistic and continuum realms has successfully simulated three-dimensional (3-D) dislocation loop nucleation, growth and interaction, a classical problem in the theory of dislocations.

This paper aims to demonstrate the feasibility of a recently developed concurrent atomistic-continuum (CAC) methodology [15–17] to simulate the nucleation, growth, and interaction of 3-D dislocation loops in Al, Cu, and Si, three systems that exhibit distinct differences regarding dislocation dissociation and mechanisms for loop growth. The CAC method is based on the formulation originally referred to as the atomistic field theory (AFT) [18–20]. The formulation starts with a description of crystalline materials as a continuous collection of lattice cells but with a group of discrete atoms embedded within each lattice cell. As an extension of Kirkwood's statistical mechanical theory of transport processes [21,22], a field representation of balance laws is derived, which has a continuum framework at the unit cell level but retains the atomistic information, including the arrangement and interaction of atoms. Solutions of the balance equations consider both the lattice deformation and the rearrangement of atoms relative to the lattice. Different from most existing coarse-grained models [23], the representation of the complete balance laws makes the AFT applicable to dynamic and nonequilibrium processes, with the force field being the only empirical input. The underlying atomistic system is achieved by discretization of AFT in the limit to primitive unit cells. Assuming the collective motion of unit cells, the majority of degrees of freedom of an atomistic system can be eliminated. This thus naturally leads to a concurrent atomistic-continuum methodology.

For relatively low defect densities and dissipation due to dislocation nucleation and motion, the temperature rise should not be significant. In such cases, the AFT linear momentum equation, supplemented by the atomic force field, can serve as the governing equation. This work employs the Mishin–embeddad atom method force fields [24,25] for Al and Cu, and the Stillinger–Weber cluster functional force fields [26] for Si. The governing equations are discretized with a uniform finite element (FE) mesh using a linear shape function. To mimic the unit cells of Al, Cu, and Si, we choose the rhombohedral shaped element with all the element surfaces being their $\{1\,1\,1\}$ slip planes. This allows dislocation nucleation and migration in the coarse-grained (CG) simulation. In fact, as a dislocation passes along an interelement boundary, a shear discontinuity of the Burgers vector compiles their relative displacement. If desired to more properly account for propagating core structure, several fully resolved atomistics layers can be added between coarse-grained elements. However, avoiding such an assignment is desirable and it is interesting to consider how behavior emerges from allowing the Burgers vector to effectively spread across entire interelement boundaries as the dislocation passes. Certainly the net Burgers vector is maintained, as well as associated long-range stress fields transmitted through the lattice as in discrete dislocation theory; however, mobility relations might be affected. In this work, no adaptive re-meshing is undertaken to resolve migrating dislocations. The code is parallelized and run on $N = 48$ processors, and scales approximately as $O(N)$.

Figure 1 presents the CG models of single crystal Cu, Al and Si specimens with a rhombohedral void initially introduced in the interior (Fig. 1a). The dimensions of the voids are $8.32\,\text{nm} \times 8.32\,\text{nm} \times 32.32\,\text{nm}$ in Cu, $9.32\,\text{nm} \times 9.32\,\text{nm} \times 36.21\,\text{nm}$ in Al and $12.28\,\text{nm} \times 12.28\,\text{nm} \times 48.55\,\text{nm}$ in Si. To induce the nucleation of dislocation loops within the nanoscale specimen, four ~2 nm diameter rigid spherical precipitates labeled as A–D are also introduced at the corners of the void. These precipitates interact with the surrounding environment based on the same potentials as used for the surrounding domains. The dislocations always nucleate from the edges (AB and CD) of the voids, and the dislocation lines are effectively pinned at the rigid precipitates. In this way, semicircular dislocation loops can form and grow. A side view of the FE mesh of the middle cross-section of the CG model is shown in Figure 1b. The distance between the precipitates are $d_{AB} = d_{CD} = 32.32\,\text{nm}$ in Cu, $d_{AB} = d_{CD} = 36.21\,\text{nm}$ in Al and $d_{AB} = d_{CD} = 48.55\,\text{nm}$ in Si. The front view of the CG model with the displacement-controlled boundary conditions applied on the two ends of the specimen is shown in Figure 1c. The displacement (Cu and Al under tension; Si under compression) is applied at a constant velocity of $2\,\text{m s}^{-1}$ and the resulting strain rate is $10^7\,\text{s}^{-1}$ in the present CG models. The time step employed in the simulations is 5 fs. The primitive cell arrangements for face-centered cubic (fcc) Cu and Al are shown in Figure 1d, and that for the diamond Si lattice is shown in Figure 1e. Inter-element boundaries for Cu and Al are coincident with $\{1\,1\,1\}$ slip planes, whereas they follow shuffle set planes in the Si structure. This is made in accordance with current understanding

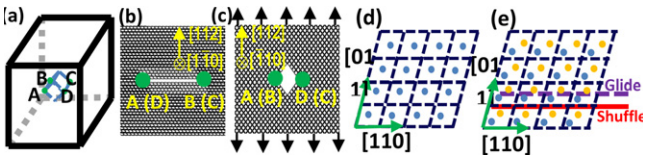

Figure 1. CG models for Cu ($50.55 \times 66.60 \times 97.66\,\text{nm}^3$), Al ($56.63 \times 74.61 \times 109.38\,\text{nm}^3$) with 43,136 elements for ~43 million atoms, and Si ($75.93 \times 100.04 \times 146.69\,\text{nm}^3$) with 43,136 elements for ~86 million atoms: (a) samples with an initially introduced rhombohedral-shaped void with rigid spherical precipitates labeled as A–D, (b) cross-section of the CG model, (c) loading conditions in the $\langle 1\,1\,2\rangle$ direction, (d) the $(1\bar{1}1)$ projection of the fcc structure and (e) the $(1\bar{1}1)$ projection of silicon diamond structure. Each lattice cell represents a primitive cell.