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A hierarchical thermo-mechanical multi-scale technique for modeling of edge dislocations in nano-crystalline structures

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ABSTRACT

In this paper, a hierarchical multi-scale technique is developed to investigate the thermo-mechanical behavior of nano-crystalline structures in the presence of edge dislocations. The primary edge dislocations are generated by proper adjustment of atomic positions to resemble discrete dislocations. The interatomic potential used to perform atomistic simulation is based on the Finnis-Sinclair embedded-atom method as many-body potential and, the Nose-Hoover thermostat is employed to control the effect of temperature. The strain energy density function is obtained for various representative volume elements under biaxial and shear loadings by fitting a fourth order polynomial in the atomistic level. The material elastic constants are calculated by evaluating the second derivatives of the total potential energy per unit volume with respect to strain components. The evolutions of yield stress, elastic constants and bulk modulus are derived for nano-crystals of magnesium with hcp atomic structure containing different number of edge dislocations at various temperature levels. In order to provide a relation between various quantities in nano-scale level to their counterparts in macro-scale level, the material properties obtained from molecular dynamics simulations are transferred to the Gauss points of finite element mesh using the calculated strain energy function. The numerical results clearly demonstrate the behavior of material in the presence of edge dislocations at various temperatures.

1. Introduction

There are different types of imperfections and defects in crystalline structures, which can appreciably affect their mechanical properties. Numerous investigations have been performed to study the mechanical and thermo-mechanical behavior of crystalline structures in the last few decades. Dislocations are known as one of the most important classes of crystallographic defects or irregularities [1]. The presence of defects such as vacancies, impurities and cracks leads to stress concentration and ultimately causes the generation of dislocations [2]. Hence, the study of dislocation effects is important for understanding the mechanical behavior of crystalline structures at atomic level [3]. Among various methods, the molecular statics (MS)/molecular dynamics (MD) [4] and Monte Carlo (MC) [5] are the most widely used techniques for modeling the mechanical behavior of nano-materials. In molecular statics, the atomic system is modeled at its relaxed configuration, and the equilibrium state is achieved by minimizing the total energy. While in molecular dynamics and Monte Carlo methods, the positions of atoms are strictly dependent on time, and the complete response of the system can be obtained comprising of mechanical and thermo-dynamical properties of nano-materials. There are various applications of molecular statics (MS) and molecular dynamics (MD) methods in the analysis of nano-materials [6]; crack propagation [7], dislocation motion [8], influence of initial dislocation density on size effects [9], mechanical properties of defect-free metallic nano-crystals [10] and influence of cobalt impurities in the emission of dislocations [11] are noteworthy. Davydov et al. [12] performed a molecular statics study to compute the elastic properties and bulk modulus for copper at zero temperature. Davoodi et al. [13,14] investigated the effect of palladium impurities on thermal and physical properties of copper crystals, such as the elastic constants, bulk modulus, melting point, cohesive energy, isobaric heat capacity, and thermal expansion coefficient at different temperatures.

Evidently, many researchers take advantage of molecular dynamics (MD) to simulate the behavior of materials at nano-scale level. However, due to the tremendous increase in computational effort using molecular dynamics (MD), the direct atomistic simulation of a system is impractical. On the other hand, continuum based approaches such as finite element (FE) or mesh free methods

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[15] cannot model the complex interactions between atoms. Hence, the multi-scale methods based on bridging between the lower scale and the upper scale have been developed to overcome the aforementioned drawbacks. Basically, multiple scale approaches have been classified in two principal categories of *hierarchical* (or *sequential*) and *concurrent* (or *parallel*) methods [16]. In the hierarchical modeling technique, the intrinsic characteristics of smaller scale are captured and utilized as a source of parameters inputted to the boundary value problem at larger scale and vice versa [17]. In the concurrent multiple scale method, the whole domain is decomposed into various sub-domains which are coupled via transition zones or handshaking areas [18,19]. The atomistic-continuum coupling techniques are categorized into two approaches; the first approach is energy-based, in which the total potential energy of the whole system is estimated as the sum of the energies of its constituent parts and, the second approach is force-based, which is independent of the notion of a well-defined potential energy [20]. The quasi-continuum (QC) method is one of the energy-based multi-scale approaches proposed by Tadmor et al. [21] to analyze two-dimensional solid structure with defects. Knap and Ortiz [22] employed the quasi-continuum multi-scale method in three-dimensional problems. Zhang and Ge [23] presented a new quasi-continuum model, in which both the bond stretch energy and the rotational energy were used to explore a new formulation for modeling anisotropic crystalline solids. Ponga et al. [24] proposed a novel quasi-continuum multi-scale method to investigate the dynamic growth of nano-voids and the nucleation of dislocations in pure single crystals of copper under various volumetric strain rates. As other energy-based homogenization approaches, the Coupling-Length-Scale (CLS) and Bridging-Domain (BD) methods are noteworthy. Broughton et al. [25] proposed the CLS algorithm for coupling scales at finite temperature; they introduced the Tight-Binding (TB) regions to couple the atomistic domain to quantum mechanics as well as the continuum domains. In their method, the size of the finite element mesh is selected equal to the lattice constant for eliminating spurious wave reflections at MD/FE interface [26]. In the bridging-domain (BD) approach, the connection between atomic and continuum domains can be established via blending of energy in overlapping regions. Liu et al. [27] investigated the validity of bridging-domain theory for nonlinear problems such as the bending of quasi-static nanotube, and buckling and dynamic fracture in hexagonal and FCC crystals. Anciaux et al. [28] utilized the bridging-domain method for analyzing contact problems at nano-scale level. Shilkrot et al. [29,30] proposed a technique to combine quasi-continuum with continuum defect model, which is similar to discrete dislocation (DD) approach. The Generalized Particle method (GP) is introduced based on an extension of the molecular dynamics method, in which the total domain is divided into several parts containing particles of different scales [31]. Fan et al. [32] proposed the generalized particle (GP) method for seamless transition and propagation of dislocation among different scales.

In fact, it is impractical to model imperfections, dislocations and voids within the continuum mechanics using the sole application of MD or MS. Modeling the movement of dislocations and their interactions via the Molecular Dynamics analysis can consume a great deal of computational resources. An alternative technique that can be used efficiently to model the movement of dislocations is the Dislocation Dynamics (DD) method. Unlike the molecular dynamics in which the particles constitute the medium, in dislocation dynamics approach the particles are the defects which are distinct from the medium itself. The solid is almost treated like an ether through which the dislocations propagate [33]. The idea of dislocation dynamics was proposed by Amodeo and Ghoniem [33,34] as early as 1990. They presented the methodology and its application to the formation of persistent slip bands, planar arrays and dislocation cells. Po and Ghoniem [35] presented a variational formulation for constrained dislocation dynamics coupled with the heat and vacancy diffusion. Akarapu et al. [36] investigated the size dependent deformation of Cu single crystal micropillars subjected to uniaxial compression using a Multi-scale Dislocation Dynamics Plasticity (MDDP) approach. Martinez et al. [37] developed a nodal dislocation dynamics model to simulate plastic processes in fcc metals. Their model accounts for all slip systems and Burgers vectors observed in fcc systems. Huang et al. [38] used the Discrete Dislocation Dynamics (DDD) approach to model the deformation of nickel-based single crystal superalloys with a high volume fraction of precipitates at high temperature. Zhou and LeSar [39] employed 3D discrete dislocation dynamics simulations to investigate the size-dependent plasticity in polycrystalline, free standing, thin films. Khraishi et al. [40] presented 3D dislocation dynamics simulations to capture the interaction between gliding dislocations in a ductile metallic matrix and nearby dispersed spherical particles. Gao et al. [41] employed the 3D dislocation dynamics to study the influence of misfit stress on dislocation glide in single crystal superalloys. Weygand et al. [42] modeled the size-dependent flow stress in uniformly loaded pillars using discrete dislocation dynamics simulations. Yasin et al. [43] developed a finite element framework to couple continuum elasto-viscoplasticity with the 3D discrete dislocation dynamics to simulate the deformation of single crystal metals (fcc and bcc) of finite domains taking into account the size and boundary effects. Obviously, a propoer integration algorithm is an ingredient part of numerical simulations of dislocation dynamics. Recently, Sills et al. [44] developed an efficient time integration scheme for simulating dislocation dynamics of work hardening.

Coupling atomistic-continuum method is one of the most popular approaches proposed by researchers based on the CB hypothesis to model dislocations in continuum mechanics. The basic assumption in the CB hypothesis is that when the atomic structure is subjected to a homogeneous deformation gradient on its boundaries, all atomic positions experience the same deformation as specified by the deformation gradient [45]. Khoei et al. [46] studied the validity of CB hypothesis by directly comparing the results of MD simulations and CB hypothesis using the Sutton-Chen many body potential. Qomi et al. [47] developed the Boundary Cauchy-Born method to capture the surface effects by introducing the surface, edge and corner elements. Khoei et al. [48] proposed the modified boundary Cauchy-Born method to properly model the surface effects in nano-crystalline structures. Khoei and Jahanshahi [49] employed the modified Cauchy-Born method to develop a plasticity model at nano-scale level by decomposition of the deformation gradient $\mathbf{F}$ into plastic part $\mathbf{F}^p$ and elastic part $\mathbf{F}^e$, i.e. $\mathbf{F} = \mathbf{F}^p\mathbf{F}^e$ that was in contrast to conventional decomposition of $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$ usually encountered in the literature. Khoei et al. [50] proposed the modified Cauchy-Born method to investigate the validity of CB hypothesis in stress space when the homogeneity of deformation gradient is not preserved. Khoei and Ghahremani [51] developed the temperature-related Cauchy–Born hypothesis to capture the temperature effect in addition to surface effects. Ghaffari et al. [52] investigated the surface effects in three-dimensional case with complex geometry via finite element and modified boundary Cauchy-Born method.

In the present study, a hierarchical multi-scale model is developed to study the role of temperature and primary edge dislocations on mechanical properties of nano-materials, such as elastic constants, bulk modulus and yield stress of hexagonal atomic structure. The nano-crystalline material used here is magnesium (Mg) whose atomic structure is of *hcp* type. In order to carry out the multi-scale analysis, two dimensional representative volume elements (RVEs) are assumed to coincide with top layer of atoms in