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Coarse-grained elastodynamics of fast moving dislocations

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ABSTRACT

The fundamental mechanism of dynamic plasticity in metallic materials subjected to shock loading remains unclear because it is difficult to obtain the precise information of individual fast moving dislocations in metals from the state-of-the-art experiments. In this work, the dynamics of sonic dislocations in anisotropic crystalline materials is explored through a concurrent atomistic-continuum modeling method. We make a first attempt to characterize the complexity of nonuniformly moving dislocations in anisotropic crystals from atomistic to microscale, including the energy intensities as well as the wavelengths of acoustic phonons emitted from sonic dislocations, and the velocity-dependent stress fluctuations around the core of nonuniformly moving dislocations. Instantaneous dislocation velocities and phonon drag effects on the dislocation motions are quantified and analyzed. Mach cones in a V-shaped pattern of the phonon wave-fronts are observed in the wake of the sonic dislocations. Analysis of simulation results based on a wavelet transform show that the faster a dislocation is moving, the longer the emitted phonon wavelength. The dislocation velocity drops dramatically with the occurrence of the interactions between dislocations and phonon waves reflected from the boundaries of specimens. The concurrent atomistic-continuum modeling framework is demonstrated to be the first multiscale method that explicitly treats the strong coupling between the long-range elastic fields away from the dislocation core, the highly nonlinear time-dependent stress field within the core, and the evolutions of the atomic-scale dislocation core structures. As such, it is shown that this method is capable in predicting elastodynamics of dislocations in the presence of inertia effects associated with sonic dislocations in micron-sized anisotropic crystalline materials from the atomic level, which is not directly accessible to the recent elastodynamic discrete dislocation model.

1. Introduction

Dynamic failure studies of materials under high strain rate loading conditions generally fall into two major categories [1,2]: dynamic fracture and dynamic plasticity. Dynamic fracture deals with the creation of new surfaces resulting from the creation of displacement discontinuities at a fraction of speed of sound in materials [2–5]. Dynamic plasticity studies relate the dynamic dislocation and/or twinning-mediated response of solids to the imposed loading at high strain rates [1,6]. Issues considered in dynamic plasticity typically include the mobility of dislocations in crystals, evolutions of dislocation density and structures, rate-controlling mechanisms of plastic flow, and so on. In particular, the plastic shearing rate for each slip system in a crystal is usually determined via the Orowan equation as the product of dislocation density, mean velocity [7], and Burgers vector. Although the dynamics of dislocations [8–14] has been the subject of intense studies for decades, the complexity of dislocations moving near and above the sonic velocity in crystals remains relatively lightly explored. The associated physical phenomena are not yet completely understood.

Extensive experiments [15–17] have successfully captured the motion of dislocations in materials under external loading, however, current experimental investigation of dynamic behavior of an individual dislocation in metallic solids is a daunting challenge due to the angstrom-scale core structure and the characteristic THz-

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level frequencies of the localized lattice vibrations associated with the fast moving dislocations. Direct experimental observation of sonic dislocations in solids was not possible until an alternative material, a plasma crystal, was recently developed [18–20]. Given that the inter-particle distance in plasma crystals is on the order of 100 μm or above, characteristic frequencies are on the order of 100 Hz or below, and the speed of sound in a plasma crystal is on the order of 10 mm/s [19], experiments on plasma crystals can provide qualitative understanding of dynamic behavior of sonic dislocations in certain solids [20]. However, such experiments cannot provide precise information regarding the velocity, acoustic phonon emission, or core stress fields of fast moving dislocations in crystalline metals.

In addition to experimental measurements, various theoretical models describing dislocation motion in materials have also been developed in the past 80 years. Theoretically, the physics of fast moving dislocations is complicated due to the strong coupling between the highly nonlinear short-range atomic-scale core stress fields and the long-range linear elastic stress field in the medium away from dislocation cores. Pioneering linear elastic models such as the well-known Peierls model [21], the Peierls–Nabarro model [10] or the Eshelby-Frank-Nabarro model [22] have contributed basic understanding but have ignored the nonlinearity, nonlocality, and the lattice discreteness in dislocations [7,23]. Under such simplifications, the classical Peierls model is believed to lack a drag mechanism which provides the resistance to be overcome by the applied stress to maintain dislocation motion [24]. Consequently, this model fails to predict a reasonable kinetic relation between the applied stress and dislocation velocity in materials. Such a drawback in the original Peierls model has served to motivate extensive development of increasingly sophisticated extended Peierls models [13,24–28], such as the one enhanced with a kinetic relation to include some notion of discreteness of the core structures [24]. These extended Peierls models are widely used and playing crucial roles in modeling dislocation plasticity in materials. Despite the popularity, they still account for viscous drag and the dislocation core structure in a phenomenological way, and have very limited predictive capability.

Fortunately, modern computing resources have enabled fully atomistic simulations to be employed to capture many features of dislocations, including core structures [29], migration barriers [30–34], and junction structures [35]. For fast moving dislocations, Gumbsch and Gao [36] performed the first MD simulation of stable subsonic, transonic and supersonic dislocation motion in bcc tungsten. Since then, MD simulations have been widely used to investigate the atomic-scale physical nature of sonic dislocations [37–43]. Nonetheless, existing MD simulation results are found to have significant uncertainty due to the inherent length and time scale limitations. For example, the dislocation velocity from a simulation with a smaller MD cell size was found to be slower than that from a simulation with a larger MD cell size [44]. It was also shown that a steady-state dislocation velocity in MD can be achieved only after dislocations have interacted with several reflected stress waves from the MD sample borders [45]. Although atomic-scale simulations have been very useful in elucidating the qualitative behavior and mechanisms of mobile dislocations, it is still perhaps too early to expect the establishment of the direct quantitative connections between atomistic simulations and experiments. Given the characteristic nm length scale of a dislocation core and much longer range elastic interactions with the other dislocations, the dynamic behavior of dislocations is patently multiscale. Concurrent methods that link atomistic and continuum plasticity within one model are therefore necessary to capture the interactions among the different scales in dislocation dynamics. Over the last 20 years, numerous concurrent methods have been developed to seek atomic [46–49] and even quantum level resolution [50] at a significantly lower computational cost than that offered by just MD or ab initio calculations. For example, a finite-temperature quasicontinuum approach within the framework of maximum-entropy non-equilibrium statistical mechanics has been developed [51–53]. Although the finite temperature quasicontinuum approach has been recently applied to predict dislocation velocities in materials under dynamic loadings [52], a set of phenomenological kinetic equations of the Onsager type [54–56] for heat dissipation associated with moving dislocations has been employed.

Overall, existing theoretical and computational models do not have sufficient generality to predict all three key physical aspects of moving dislocations: 1) evolution of atomic-scale core structures; 2) coupling between the highly nonlinear short-range core stress field and the long-range linear elastic stress field away from the core; 3) material inertia associated with sonic dislocations. The current study employs a concurrent atomistic-continuum (CAC) methodology [57–67] for multiresolution modeling, based on an atomistic field formalism [68–70] in which the microscopic balance equations are formulated as an extension of Irving–Kirkwood formalism [71]. In CAC, the finite element (FE) method is used to solve for the atomic displacement field in crystalline materials. The CAC method [57–67] has naturally resulted from the employment of the uniform coarse FE mesh. By embedding the local atomic structure within each material point, CAC simulations are able to reproduce dislocation nucleation and migration in materials [61–64,72]. In addition to dislocations, CAC models are also demonstrated to be capable of reproducing the full sets of phonon dispersion relations in anharmonic polyatomic crystals [66,67]. Therefore, in principle, the CAC model admits the essential dynamics of moving dislocations on length and time scales ranging from the atomic to the mesoscopic levels of microstructure and initial-boundary value problems of interest. These features distinguish the CAC method from the microcontinuum theories [73] or the other existing multiscale methods [74] and motivates application of this method to analyze sonic dislocation behavior. Comparing to our previous CAC-based studies [57–67], the novel aspects of CAC employed in this work include: 1) Quadrilateral-shaped elements are employed to discretize the 2D fcc solid, while constant strain triangular elements and hexagonal rhombohedral-shaped elements are used in the previous CAC models of fcc crystals; 2) An algorithm based on the phonon wavelet transform is developed and implemented into CAC to quantify the instantaneous wavelength, frequency and energetics of phonon waves emitted from the moving dislocations. In addition, the local kinetic temperature rise due to the fast moving dislocations is quantified in anisotropic crystalline materials.

2. Methodology and computational specimen configuration

Here we explore the complex dynamics of fast moving dislocations by considering an idealized two-dimensional (2D) lattice which resembles the atomic configuration of a fcc single crystal (Fig. 1a). Plane strain conditions are considered; atoms are not allowed to move along the $\boldsymbol{z}$-direction and are free to move in the $\boldsymbol{x}$ and $\boldsymbol{y}$ directions. The 2D models, instead of quasi-2D or 3D models, are constructed and investigated for two reasons: 1) the only existing direct experimental observation of sonic dislocation motions in solids is in 2D plasma crystals; 2) the dislocation lines in three dimensions are curved and therefore of mixed character, having both edge and screw components. The dynamics of mixed mode dislocations in an anisotropic crystal will be rather complicated because the contributions to core radiation from the edge and the screw components are strongly coupled. Thus, the 2D