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Effects of phonons on mobility of dislocations and dislocation arrays

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ABSTRACT

This work presents a coarse-grained atomistic study of the effect of phonons on the mobility of edge dislocations. A variety of phenomena, including phonon focusing and phonon-induced dislocation drag, are reproduced in the simulations. Results show that interaction with phonons slows down the dislocations and phonon focusing results in the arrest of dislocations. A wavelet analysis, together with visualization, reveals that the phonon-dislocation interaction leads to a reduction of the energy associated with the dislocation core, with some energy lagging behind the decelerated dislocation or dispersed around the arrested dislocation through emission of secondary phonon waves, thus clarifying the underlying physics.

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Dislocations are line defects that play a significant role in both the mechanical and thermal transport behavior of crystalline materials. In crystalline materials with a small Peierls barrier (intrinsic lattice resistance), for example, (111) slip planes in FCC crystals, phonons are believed to be the primary sources of damping for dislocation motion in an otherwise perfect lattice [1]. However, the glide behavior of mobile dislocations is extremely difficult to probe [2], and the "otherwise perfect lattice" can never be achieved under actual experimental conditions. Other lattice defects such as impurities, vacancies, dislocation tangles and grain boundaries also interact with dislocations, complicating investigation of phonon-dislocation interactions. Moreover, the study of the dynamic process of phonon-dislocation interactions requires high fidelity in the time domain. Significant efforts have been devoted to modeling the interaction between dislocation and waves. Pioneering works have largely considered drag effects under overdamped conditions within the context of linear elasticity of isotropic solids [3–7]. Most recent developments have accounted for the material anisotropy [8,9]; however, these studies have considered either static or quasi-static conditions. The mean distance between multiple dislocations was assumed to be large, effectively decoupling interactions [10]. During the past few decades, molecular dynamics (MD) simulations have been useful in fostering more predictive understanding of the dynamic behavior of dislocations and phonon-defects interactions at full atomic resolution [11,12]. However, the long-range nature associated with the phenomenon of interaction of phonons with fast moving dislocations is usually beyond the length scale limit of MD at reasonably affordable computational cost.

In this work, we perform coarse-grained atomistic simulations to investigate the effect of phonons on moving dislocations using the concurrent atomistic-continuum (CAC) method [13–15]. The CAC method was inspired by the statistical mechanical theory of transport process by Irving and Kirkwood (IK) [16,17]. In CAC, a crystalline material system is described as a continuous collection of material points, each representing a lattice cell; embedded within each material point is a group of discrete atoms [18–20]. As a methodology derived bottom-up from atomistics [21], CAC requires no priori empirical rules or parameters other than the interatomic force field, the same as required by MD. With the interatomic potential being the only constitutive relation, CAC naturally reproduces the complete set of the dispersive phonon relations [22,23]. It is well known that MD cuts off phonons with wavelengths greater than the size of the periodic simulation cell [24,25]. In contrast, CAC cuts off short wavelength phonons by coarse-graining and, as demonstrated in our previous work [23,26,27], can predict the dynamics of long-wavelength phonons, with the minimum wavelength determined by the size of the finite element. If modeled at full atomic scale resolution, CAC can exactly reproduce the dynamics of an atomistic systems [27]. In addition, the CAC method has been successfully applied to quantify dislocations motion [28]. At the nanoscale, those CAC results have been compared with atomistically resolved MD simulations for validation. It was shown that the dynamic behavior of dislocations and emitted phonons from the CAC simulations are quantitatively comparable with those from MD simulations. Therefore, the CAC method is used in this work to study the dynamics of the moving dislocations and the interaction with medium- and long-wavelength phonons.

To simulate the transient response of crystalline materials to ultrashort laser pulses that are widely used in various experiments [29–33], a phonon representation of heat pulses, termed a coherent phonon

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pulse (CPP), has been developed [34]. The CPP model mimics the coherent lattice excitations arising from ultrafast laser pulses and facilitates the analysis of phonon wavelength-dependent material behavior as well as the visualization of the transient processes of phonon scattering [34]. One of our recent works has demonstrated the capability of CAC method using the CPP model with a Bose-Einstein distribution to predict the dynamics of long-wavelength phonons and their interactions with grain boundaries [27]. In this work, we employ the same approach to study the effect of long-wavelength phonons on moving dislocations in a 5.2 μm × 5.2 μm L-J solid [35] that contains ~0.5 billion atoms. The details of the interatomic potential employed, as well as the dynamic behavior of dislocations in this material, have been presented in our previous works [28]. To generate dislocations, a shear loading is first applied to deform the sample to produce a global shear strain $\gamma = 0.01$ in the specimen; then local shear displacements are applied near the initially introduced notches on the left edge of the specimen to nucleate dislocations. After the dislocations nucleate, the loading boundaries are frozen, and the dislocations are allowed to propagate spontaneously without continuous loading, driven by the high shear stress field in the specimen. The heat pulse is then applied at the center of each specimen, and subsequently, the nonequilibrium phonons propagate freely towards the moving dislocations. The wave speed of the longitudinal acoustic (LA) and transverse acoustic (TA) phonons near the Γ-point (the long wavelength phonons) are measured to be ~6700 m/s and ~3900 m/s, respectively. In this work, no thermostat is applied to the system, which starts at 0 K. This serves to isolate the understanding of the behavior of phonons emitted from dislocations as well as phonons excited by the propagation of the heat pulse from the thermal motion of atoms associated with an imposed finite background temperature. The dislocation-phonon scattering, the phonon-phonon scattering, the local temperature generated by the heat pulse, and the scattering behavior naturally emerge as a consequence of the governing equations and interatomic potential, without the assistance of heat diffusion associated with thermostatting.

Fig. 1 presents the simulation results for the motion of a single edge dislocation and an array of edge dislocations in a single crystal. Fig. 1(b) and (c) show the kinetic energy distribution during the nucleation and migration of a single dislocation and multiple dislocations, respectively. It is seen that the motion of dislocations is accompanied by radial-shape wavefronts of phonons ahead of the moving dislocations, as well as V-shaped wave tails in the wake of the dislocations. Fig. 1(b) shows that the radial wavefronts propagate faster than the dislocation core, indicating the dislocation is moving subsonically, with its velocity lower than the speed of sound in this material. In contrast to the case of a single mobile dislocation in Fig. 1(b), in Fig. 1(c), due to the interaction between neighboring dislocations, both the radial-shaped wavefronts and V-shaped tails of phonons accompanying each moving dislocation are scattered by the phonons emitted from the adjacent dislocations. The radial wavefronts of all dislocations interfere to form a band in front of the dislocation array (as indicated by the white dashed line), which widens as the dislocations advance. Note that the top three figures in Fig. 1(b) and (c) focus on the vicinity of a moving dislocation, while the figure located at the bottom presents the overall view of the entire crystal. We then take the first derivative of dislocation position-time history and calculate the instantaneous velocity of the dislocation; the result is presented in Fig. 1(a). For the case with multiple dislocations, we take the average velocity of all dislocations. Based on the dislocation velocity-time history, we can identify a plateau of dislocation velocity at around 3500 m/s, which is around $0.9c_T$, c_T being the group velocity of transverse acoustic phonon near Γ-point. This result is quantitatively consistent with our previous work [28], and also agrees with the observation that the dislocation core moves slower than the transverse wavefronts in Fig. 1. In addition, we find that the multiple dislocations accelerate significantly faster than a single dislocation before they reach a velocity plateau at a similar value. Fig. 1(a) also shows that dislocations travel hundreds of nanometers (dislocation array) to microns

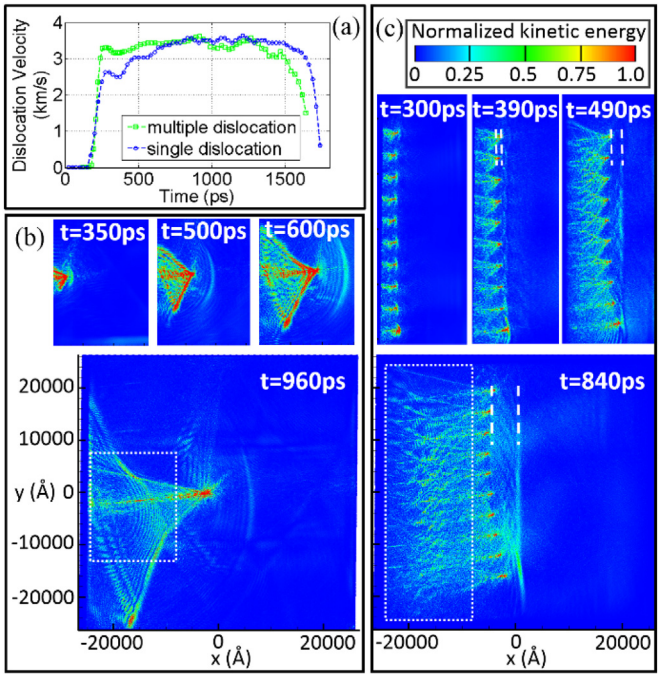

Fig. 1. CAC simulation results for (a) the motion of a single edge dislocation and multiple edge dislocations, (b) comparison of instantaneous dislocation velocities between the cases of single and multiple dislocations, and (c) the time sequence of snapshot of kinetic energy distribution in specimens showing the lattice waves associated with the nucleation and propagation of single and multiple dislocations. Note that the top three figures in Fig. 1(b) and (c) focus on the vicinity of moving dislocations, the focused regions are marked by the white dotted-line boxes in the bottom figures, which present the overall view of the entire crystal.

(single dislocation) before their velocities reach the steady state condition. This may explain why a MD simulation with modest computational resources results in a size-effect induced by the relatively small periodic simulation cell at the nanoscale [24,25]. For example, a previous work [36] conducted MD simulations of edge dislocations moving in a BCC crystal, and showed that dislocations can move at different velocities, and that shock waves can form at a fast moving dislocation. However, the longest distance the dislocations could travel in their simulations was only on the order of tens of nanometers; it was suggested that a proper system-size scaling analysis may help to investigate size effects in the atomistic model.

Fig. 2 presents simulation results of a single and multiple moving dislocations interacting with a propagating coherent phonon pulse that is applied for 10 ps at $t = 500$ ps in the simulation of single dislocation and at $t = 405$ ps in the simulation of multiple dislocations, respectively. It is noticed that the ballistic phonon wavefronts from the CAC simulations do not exactly conform to a circular shape, but rather channel along the [112] crystal directions; this results in phonon-focusing "caustics" associated with directions with especially high phonon fluxes. Fig. 2(a) presents the time sequences of three selected snapshots of kinetic energy distribution in space, depicting the motion of a single dislocation and its interaction with the phonons in the pulse, with the curves comparing the dislocation velocity from simulations with and without the imposition of the phonon pulse. It is seen from Fig. 2(a) that before the dislocation meets the imposed phonon pulse, the two dislocation velocity curves overlap; then at around $t = 785$ ps, there is a sudden decrease on the one with phonon pulse (red), and a recovery afterwards. By investigating the details of the dynamic process, we find that when the dislocation first meets the longitudinal phonon wave-front (one of the LA and TA focusing directions that will affect the motion of dislocations are marked by dashed line on the stress distribution in Fig. 2(a)), there is no noticeable deceleration; the direction of motion of the dislocation deviates from the longitudinal phonon focusing direction. However, the

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