Computational Materials Science 124 (2016) 259–266

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Harmonic effects in atomistic phase interactions between phonons and dislocations moving at relativistic velocities

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ARTICLE INFO

Article history:
Received 9 February 2016
Received in revised form 31 July 2016
Accepted 1 August 2016
Available online 11 August 2016

Keywords:
Linear elastodynamics
Transonic
Phonon scattering
Peierls-Nabarro
Supersonic
Transverse wave
Molecular dynamics
Copper

ABSTRACT

The observation of distinct velocity ‘plateaus’ below the upper limits of the sonic velocity have frustrated many in the scientific community studying high-velocity dislocation dynamics. Liebfried and Frank derived the well-established elastic models of dislocation motion, showing dislocation core energy approaches a relativistically infinite level at the limiting sonic velocity due to a singularity. Eshelby predicted the possibility of a single stable ‘transonic’ velocity with the Peierls-Nabarro model, however he could not provide a physical mechanism to explain the acceleration from the sub-sonic velocity limit. Weiner proposed a linear elastic model where the atomic masses within a dislocation move in a coordinated (or harmonic) manner due to coupled momentum transfer, and used this to predict the limiting velocity at 0 K. In modern times, detailed phonon dissipation models have been developed to predict the dislocation velocity relationships at higher temperatures. However, few studies have been performed to show how phonon interactions with dislocations influence the atomistic behaviour. This paper presents a conceptual model based on the coupled motion of multiple atoms in the dislocation core. When compared with molecular dynamics simulations, the model predicts key qualitative and quantitative metrics, such as the lower and upper limiting dislocation velocities. Detailed atomistic analysis confirms the in-phase coordination of atoms that become disrupted by interactions with dislocations at both limiting velocities. The model provides a physically realistic mechanism that is capable of explaining the observation of subsonic and transonic velocity plateaus.

1. Introduction

The stress-velocity relationship of dislocations has been described with simplified linear elastic ‘coupled-spring’ models since the early 1960s, in terms of the displacement on a one-dimensional row of atoms caused by a propagating shear wave (dislocation) [1,2]. In such models, atoms are initially placed at the equilibrium lattice sites in a linear orientation, and are only able to be translocated up to a peak potential or to the minimum of the energy well. These models predict that the linear relationship between the stress and the steady-state velocity will ‘break-down’ when the velocity is high enough to cause an atom to cross the saddle point of the potential energy surface and enter the adjacent energy well [3]. This provides a physically-realistic mechanism for dislocations approaching an asymptote at a subsonic limiting velocity. It also explains the break-down of the singular dislocation core at relativistic velocities approaching sonic limits. However, the simplification into a one-dimensional spring model ignores temperature effects that cause thermal vibrations, phonon interactions and vacancy interactions. Hence, the suitability of such models for explaining relativistic dislocation velocity effects in non-static conditions cannot be predicted with simplified spring models.

In 1956, Eshelby derived an analytical solution which predicted a stable super-sonic dislocation velocity could be obtained at $\sqrt{2}$ times the transverse velocity of sound (C_{tr}); however at the time this was considered little more than a theoretical curiosity [5]. In fact, it was considered to be physically impractical or impossible to reach velocities exceeding the sonic limit, and despite a mathematical solution existing, there was no physical mechanism proposed to explain this [6]. However, modern-day molecular dynamics (MD) simulations of dislocations at high temperature and stress regularly describe the observation of several discrete supersonic dislocation velocities [6–10]. These are commonly referred to as transonic or supersonic velocity regimes; however the observation of steady-state motion at velocities above the longitudinal speed of sound (C_l) has not been confirmed [8].

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http://dx.doi.org/10.1016/j.commatsci.2016.08.001

The present study analyses the atomistic phase-velocity effects with high-fidelity atomistic simulations of dislocations moving at relativistic velocity in a dipole configuration at 300 K, using modern inter-atomic potentials. It is noteworthy that computationally-intensive simulations with rigorous stress-control regimes were a key pre-requisite to study dynamic effects [4]. The investigation was motivated by the observation of transient stacking fault width observations and multiple velocity plateaus, during a recent assessment of the impact of dislocation core width on the dislocation mobility in pure FCC copper. These results showed that the stacking fault width, phonon drag and (by association) core width were impacted as the velocity approached the sonic limits. This was explained because the 'narrow' dislocation core is conventionally believed to cause the substantial majority of phonon drag effects at high velocity [11]. It is noteworthy that the model being proposed does not involve an analytical approach based on elastic theories of Liebfried [12], Eshelby [5] or Nabarro [13]. The conceptual framework is only based on atomistic behaviours in terms of qualitative and quantitative simulation results. For this reason, the results may also help to elucidate the remaining 'discrepancies with simulations' where the analytically predicted plateau velocities are substantially higher than simulation results [14].

Caro and Marian proposed a model in 2006 [10] which decomposes the mobility behaviour into a linear regime when the velocity is below a minimum value (C_{min}), above which radiative terms become significant. The "limiting velocities" indicate a "singularity" in the stress-velocity relationship, where the limits are influenced by C_{tr} [10]. A demarcation is made between the lower ($C_{tr,low}$) and upper ($C_{tr,high}$) transverse sonic velocity singularities, which depend on different phonon dispersion modes. The principles of the model and results obtained for C_{min}, $C_{tr,low}$ and $C_{tr,high}$ are described in this paper and used as a quantitative benchmark.

On the basis of the distinctive characteristics of the dislocation core, a simple physical mechanism is proposed which would explain the existence of several velocity plateaus, based on the principle of resonance in the coupled atomistic motion. The paper describes the conceptual framework and mechanism for the multiple velocity plateaus of dislocations, with a relevant literature review of phonon dispersion models. High-fidelity atomic simulations are used to analyse the linear vibrational motion of atoms in the direction of dislocation motion, to explicitly evaluate the disruption in the phase velocity caused by slip. The velocity of the dislocation core is evaluated independently from the atomic motion by post-processing to extract the dislocation core as a 'linear defect' from the atomistic framework [15]. By distinguishing the dislocation and atomistic phase velocities, this study investigates the 'resonance effects' within a dislocation core moving at the limiting velocities.

2. Theory

Bhate predicted that phonon-interactions with dislocations could be coincidental with the 'local modes' of dislocation motion at favourable velocities [16]. The phase velocity motion of thermally excited atoms can be described in a simplified manner by using a sinusoidal velocity profile, which will serve as a suitable approximation for the results presented. This is analogous to the Weiner model [1], which assumed that the coupled potential wells of a row of atoms can be described as a parabolic peak and trough. If the disruption in the vibrational motion caused by a dislocation is sufficient to cause an atom to leave its potential well, it will cause a knock-on effect in the adjacent atom. Such behaviour is analogous to the harmonic coordinated motion of coupled pendulums [1,2]. Weiner performed a simple computational evaluation of the linear spring model to show that the 'knock-on' effect would occur at approximately 0.7 times the transverse velocity of sound (C_{tr}). The knock-on effect resulted in core spreading, due to the compression and rarefaction in leading and trailing dislocation edges [2]. The effect of spreading extension of the dislocation core was described as a "break-down" effect [3].

At elevated temperature, the dislocation velocity is limited by the drag forces that are caused by energy dissipation from interaction with phonons (quantized sound waves [17]). At high velocities, radiative damping by phonon scattering effects is widely accepted as the dominant mechanism and will increase with the stress [6,7,18]. Although modern results indicate that radiative damping can occur at any velocity, strong deviations from linear behaviour are not apparent until the velocity approaches the sonic velocity thresholds [8,10]. Bhate et al. [16] originally claimed that phonon modes might exist which coincide with equivalent phases of dislocation glide motion, however this model does not fit well with results obtained from rigorous atomistic analysis [8]. According to Caro and Marian's model, the complexity of the phonon dissipation effect is compensated for with a sophisticated model that accounts for non-linear radiative damping effects, albeit with some assumptions [10]. In Caro's model, C_{min} was predicted from the minima of the dispersion curves for the $C_{tr,low}$ and $C_{tr,high}$ phonon curves; however these curves depended strongly on the glide direction of the dislocation line. Accordingly, for a dislocation moving in the [1 1 0] direction, it was analytically predicted that C_{min} would be ~0.34 C_l, $C_{tr,low}$ would be ~0.38 C_l and $C_{tr,high}$ was 0.65 C_l. More recently, Pellegrini obtained a convenient solution from a multi-physics, collective variable mathematical approach incorporating the effects of core-width fluctuations on the high-rate dislocation inertia [14]. On this basis, he mathematically predicted a 'bifurcated' velocity profile, with a sudden transition from 'subsonic (C_{tr})' to 'transonic (C_l)' velocity. Pellegrini's model also described the importance of arbitrary core-width variations in obtaining an accurate solution for the velocity approaching the 'transonic velocity' [14].

It is important to note that the analytical models are strongly dependent on the dislocation line orientation, which also dictates the screw or edge character of the dislocation. In FCC metals, dislocations decompose into Shockley partial dislocations with a mixed edge and screw character. For this reason, it is difficult to determine whether differences within the dislocation core also play a significant role. Despite this limiting assumption, the phonon dissipation model is well-established within the scientific community and is generally accepted to be superior for modelling relativistic velocity effects at elevated temperatures. Such models are commonly presumed to be distinct from the simplified linear spring models.

This study uses simulations to evaluate the behaviour of the atomistic medium, and hence determines whether it can be distinguished from the behaviour of a moving dislocation because of coupled momentum effects (i.e., atomistic harmonics). By simplifying the description of the atomistic motion into a group of atoms arranged in a one-dimensional chain along the direction of dislocation glide, the resonance effects caused by the 'knock-on' effect can be studied.

3. Methods

Molecular dynamics simulations were performed with the LAMMPs programme [19], in pure FCC copper that was simulated using the embedded atom method potential obtained from Ref. [20]. To capture the high-velocity dislocation dynamics, a large simulation cell with dimensions of 20.5 nm × 15.1 nm × 19.6 nm