Acta Materialia 115 (2016) 143–154

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

Phonon scattering during dislocation motion inducing stress-drop in cubic metals

Soon Kim [a], Duc Tam Ho [a], Keonwook Kang [b], Sung Youb Kim [a, *, 1]

[a] Department of Mechanical Engineering, Ulsan National Institute of Science and Technology, Ulsan 44919, South Korea
[b] Department of Mechanical Engineering, Yonsei University, Seoul 03722, South Korea

ARTICLE INFO

Article history:
Received 18 January 2016
Received in revised form
24 March 2016
Accepted 29 May 2016

Keywords:
Dislocation
Atomistic simulation
Phonon scattering
Iron
Aluminum

ABSTRACT

This work proves that scattering of elastic waves in the dislocation core induces an unusual behavior called *stress-drop*, which is defined for the first time in this study as a phenomenon where an externally applied stress drops inside a nano-sized cubic metal during dislocation motion. We develop a theoretical phonon scattering model based on discrete lattice dynamics and derive simple analytical equations to quantify the magnitude of the stress-drop. The proposed model is supported by atomistic simulations of perfect dislocations in bcc iron, where the stress-drop resulting from bond breaking is inversely proportional to the square of the dislocation speed. The derived equation is in excellent agreement with direct atomistic simulations for edge and screw dislocations. Next, we extend the equation to the edge dislocation in fcc aluminum where the dislocation exists as a stacking fault ribbon surrounded by two Shockley partial dislocations and thus the interaction between them is important. The extended equation accurately predicts the phonon scattering, resulting in the stress-drop by the oscillation of the two partials as well as bond breaking. In addition to the discussion on the validity of our model and equations at absolute zero, we investigate the temperature and size effects on our equations. As temperature increases, the magnitude of the stress-drop decreases and converges to zero even at very low temperature because of the extremely small Peierls barrier. Moreover, the magnitude of the stress-drop decreases, as the thickness of the nanoplate increases, which shows that the stress-drop is a mechanical behavior that is prominent on the nanoscale.

1. Introduction

Various experiments and theories have suggested that dislocations act as plasticity carriers. Since then, intensive studies have been carried out to understand the mechanical behaviors of a single dislocation by computer simulations [1–3] and the physical importance of it by theoretical models [4–6]. These studies have, in particular, focused on measuring mobility and Peierls stress of dislocations depending on their types. This is because they are used to characterize dislocation segments in mesoscale dislocation dynamics (DD) simulation and finally determine plastic behaviors of materials.

Numerous studies have pointed out that both the mobility and Peierls stress are strongly influenced by the core structure of dislocations [7–10]. For example, in fcc crystals, Schmid law describes their slip behaviors and Peierls-Nabarro (P-N) model also explains high mobilities and low Peierls stresses of dislocations well with their extended planar core structure and reduced Burgers vectors [7,8]. Physically, perfect dislocations in the fcc metals are dissociated into two or more partial dislocations with stable stacking fault(s) between them to reduce an elastic energy of the dislocation, so they form wide cores. Since Burgers vector is distributed widely in slip plane, the relative displacements of atoms in core to its neighbor atoms are small compared to narrow core. This requires less motions of atoms in core to translate the dislocation so the fcc crystals have small Peierls stress [7]. On the contrary, in bcc crystals, Schmid law cannot be applied because their plastic behaviors are governed by screw dislocations whose core structure is extended out of slip plane, that is non-planar core structure [8]. The non-planar spreading induces an anchoring effect to dislocation motion, which requires significant energy to translate the dislocation [7]. In addition to the non-planar structure, a compactness of the core leads the bcc crystals to have higher Peierls

* Corresponding author.
E-mail address: sykim@unist.ac.kr (S.Y. Kim).
[1] Present address: EB1 401-4, 50 UNIST-gil, UNIST, Ulsan 44919, South Korea.

http://dx.doi.org/10.1016/j.actamat.2016.05.053
1359-6454/

stress compared to the fcc crystals based on P-N model [2,7]. For covalent-bonded materials such as silicon or zinc-blende crystals, dislocations have very narrow core due to strongly directional atomic bonds and this induces extremely high Peierls stress. Especially, it was reported that reconstruction process which eliminates dangling bonds contained in the core of partial dislocations in silicon increases a resistance to their motion [9]. Not only the analysis, but there have been also several attempts to manipulate dislocation mobility by perturbing its core properties. For instance, it was observed that dislocation speed drastically increases during electronic excitation in several semiconducting crystals [10]. The enhanced mobility is because of reduction in an activation energy for dislocation motion, which is induced by phonons, emitted from the core, that force the dislocation to vibrate.

Furthermore, the dislocation core has drawn a lot of attention from many physicists and material scientists because mechanical response in this region does not follow linear elasticity theory. There are two main reasons why the linear elasticity theory cannot describe the core region. First, a strain field applied in the core is too large to use the linear elasticity theory [11]. Second, if the strain field is applied in finite region whose size is limited, an elastic response in a specific point depends not only on stress at that point but also at surrounding volume around the point, so the response is non-local. This behavior comes from discrete nature of the dislocation core [12]. Due to these theoretical difficulties, atomistic [2,13] and density functional theory (DFT) simulations [14] have been emerged as tools for deeper understanding of the core region since the late twentieth century. In addition to simulation techniques, however, theoretical descriptions of dislocation mobility have been tried by simplifying the actual core structure [4,6] or assuming piecewise harmonic interatomic potential [5].

Using atomistic simulations, it has been proved that the mechanism of dislocation motion depends on various external factors [1,15–20]. For example, $1/2<111>\{110\}$ edge dislocation in bcc crystals moves by nucleation and propagation of double-kink under low temperature [15] but it moves as a straight line at temperature higher than 100 K [16]. Compared to the edge dislocation, a kink is easier to be nucleated on a screw dislocation line in bcc crystals because it has a non-planar core structure and higher Peierls barrier than the edge dislocation [15,17]. When a dislocation moves rigidly, the mobility of dislocation is inversely proportional to temperature due to a viscous drag mechanism [16,18]. In contrast to rigid motion, when dislocation moves by a double-kink mechanism, the mobility of dislocation increases with increasing temperature because kinks are more frequently nucleated at higher temperature [19]. Based on these thermal dependences of dislocation motion, the mobility function for edge dislocations in iron was calculated [16], and the critical stress to move screw dislocation in iron was expressed as a function of temperature [20] by fitting the atomistic simulation results. Not only the temperature but also the strain rate affects the dislocation mechanism. It was reported that the mechanism transitions from smooth to rough motion of screw dislocation as the strain rate increases [1]. However, most explanations which depend solely on computational methods have shown weakness to expand their ideas to other cases due to their phenomenological approaches. This limitation can be made up for theoretical approach.

Among the theoretical methods to describe dislocation motion, the most widely used one is the discrete lattice dynamics model [21–30]. This assumes that a system consists of uniformly arrayed atoms, and displacements of the atoms are derived by solving dynamic equations of motion. Based on the model, there have been many papers to derive dislocation mobility in analytic form [18,21,26], and it allowed one to quantify drag effects induced by phonon scattering in the dislocation core on its mobility [25,26]. Several types of drag effects due to phonon scattering were reported. First, momentum transfer from thermal phonons to a dislocation forces it to vibrate by phonon scattering. However, as the dislocation vibrates, it radiates energy away to phonons. This effect is known as the *fluttering mechanism* [31]. Second, when the phonon flux is not symmetric with respect to the dislocation core, the scattered phonons transfer momentum to incident phonons in direction opposite to its motion. This effect is called *phonon wind* [21,32]. Finally, periodic changes in the core structure and irregular motion over the Peierls barrier induce *radiation friction* to dislocation motion [21,22,24,30]. This effect exists even at 0 K because it occurs purely due to lattice discreteness. The explanations of drag effects on dislocations based on a theoretical approach provide us with profound insights to understand its core, but they have an inevitable limitation in that an ideal case should be assumed to simplify the real phenomenon.

In this work, both computer simulations and theoretical modeling are carried out. We develop a phonon scattering model by assuming that the system has a simple lattice structure based on discrete lattice dynamics and prove the model by comparing it with results of atomistic simulations conducted for cubic metals. First, we derive an analytical equation to calculate the magnitude of the stress-drop for the simplest case, and then compare it with atomistic simulation results, which correspond to one when edge and screw dislocations are moving in bcc iron nanoplate and nanowire, respectively at 0 K. Second, we extend the equation to a more complex case and compare the extended equation with the result of the simulation, which corresponds to the motion of an edge dislocation in fcc aluminum nanoplate. Since the dislocation is dissociated into two partial dislocations in fcc crystals, the interaction between them should be considered. The theoretical equation obtained in bcc iron is extended to consider the oscillation effect derived from their interaction. Finally, as we control the temperature and size of the system, we observe changes in the magnitude of the stress-drop and in dislocation speed and prove the validity of the equations obtained above.

2. Computational methods

All of the atomistic simulations presented in this work were performed using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [33].

2.1. Edge dislocation

Two materials, iron and aluminum, were used to simulate edge dislocation. For iron, the embedded atomic method (EAM) interatomic potential developed by Mendelev et al. [34] was used to describe the interaction between two atoms. The principal axes x, y and z directions were oriented along the $[111]$,$[1\bar{1}0]$ and $[11\bar{2}]$ directions, respectively. The size of the simulation cell used in this study was 22.5 nm × 18.0 nm × 1.40 nm unless stated otherwise. Periodic boundary conditions were applied along the x and z directions, but relaxation was allowed in the y direction. After relaxation by the conjugate gradient energy minimization scheme, a single edge dislocation, whose Burgers vector is $\mathbf{b} = 1/2[111]$, was embedded along the z direction in the iron nanoplate by deleting the lower-half plane and applying displacement fields to the atoms. The applied displacement fields are derived in Ref. [31]. The final configuration of the dislocation core is shown in Fig. 1a. To examine the size effect, additional cells whose sizes are 44.5 nm × 36.2 nm × 1.40 nm, 66.8 nm × 54.3 nm × 1.40 nm and 89.0 nm × 72.5 nm × 1.40 nm were also used. Although lengths along the x direction were changed, the periodic boundary