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Velocity dependent dislocation drag from phonon wind and crystal geometry

Daniel N. Blaschke

Los Alamos National Laboratory, Los Alamos, NM, 87545, USA

A B S T R A C T

The mobility of dislocations is an important factor in understanding material strength. Dislocations experience a drag due to their interaction with the crystal structure, the dominating contribution at high stress and temperature being the scattering off phonons due to phonon wind. Yet, the velocity dependence of this effect has eluded a good theoretical understanding. In a previous paper, dislocation drag from phonon wind as a function of velocity was computed from first principles in the isotropic limit, in part for simplicity, but also arguing that macroscopically, a polycrystalline metal looks isotropic. However, since the single crystal grains are typically a few microns up to a millimeter in size, dislocations travel in single crystals and cross boundaries, but never actually see an isotropic material. In this work we therefore highlight the effect of crystal anisotropy on dislocation drag by accounting for the crystal and slip plane geometries. In particular, we keep the phonon spectrum isotropic for simplicity, but dislocations are modeled according to the crystal symmetry (bcc, fcc, hcp, etc.). We then compare to the earlier purely isotropic results, as well as to experimental data and MD simulations where they are available.

1. Introduction

A fundamental problem in the dynamic response of solid metals are the mechanisms contributing to the so-called drag coefficient of dislocations under high stresses and strains: Moving dislocations (curvilinear defects in the crystal structure of the metal) experience a drag due to their interaction with the crystal structure, and represent a major factor in the understanding of material strength. Hence, many dislocation based material strength models require the dislocation drag coefficient B as one of their input parameters (typically determining the dislocation glide time between obstacles), see e.g. Refs. [1–7]. B is usually assumed to be a constant (or a constant over a simple "relativistic" factor) as a fist order approximation. Hence, more insight into the true functional form of this drag coefficient could improve those models.

Several mechanisms contribute to the dislocation drag, and depending on the temperature, pressure and dislocation-velocity (or stress) regime, different mechanisms dominate [8,9]. For example, at low stresses, the dislocation mobility is limited by various potential barriers within the crystal. Such obstacles can be overcome by a dislocation either by thermal activation (if the temperature is high enough) or by high enough stress levels. When the stress level becomes "critical", i.e. high enough to easily overcome the highest potential barrier, the dislocation drag becomes viscous in character, and a significant change in the stress-velocity dependence from non-linear to approximately linear takes place. In this high stress regime, where typical dislocation speeds are within a few percent of transverse sound speed, the dominating contribution to the dislocation drag coefficient (at temperatures around and above the Debye temperature) is the dissipative effect[1] of scattering off phonons ("phonon wind").

The theory of phonon wind has a long history, being pioneered by Leibfried and others [10–14], significantly improved from first principles by Alshits and collaborators [15–17], and was nicely reviewed in Refs. [8,9] (which may also be consulted for additional references). Due to the simplicity of Leibfrieds expression for dislocation drag ($B\sim$const.$\times T$), which represents the limit of high temperature T and small dislocation velocity in an isotropic continuum, it is still used today (despite its limitations) as an empirical fitting function to extract information on dislocation mobility from discrete lattice simulations [18–20]. In these examples, the additional damping in the high velocity regime is then accounted for empirically by adding a T-independent term which grows like $\sqrt{v}$ above some threshold velocity $v > v_0$, and which is based on Eshelby's arguments [21] for screw dislocations in an isotropic continuum supplemented by an anisotropic dispersion relation. The latter term is in stark contrast to the "relativistic" factors $\propto 1/(1 - v^2/c^2)^m$ with different exponents m and a limiting (sound) speed c introduced by many authors (see e.g. Refs. [1,2,6,7] among others) based on equally empirical arguments. Thus, a better understanding of dislocation drag from first principles at high velocities and for arbitrary crystal geometries is clearly needed.

E-mail address: dblaschke@lanl.gov.

[1] Other dissipative effects, which we do not touch upon in this paper as they are subleading in the regimes we are interested in, are the so-called thermoelastic damping, the flutter effect, and the radiation damping, see Ref. [8] for details.

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For a wide range of velocities (already starting at low velocities where phonon wind is a subleading effect), the contribution to the drag coefficient due to phonon wind is roughly constant. However, at very high velocities (i.e. more than a few percent of sound speed) the drag coefficient due to phonon wind becomes velocity dependent, indicating once more a non-linear stress-velocity dependence, and it is this regime we are primarily interested in here.

Existing continuum models of dislocation drag due to phonon wind [9] assume that the dislocation velocity is much smaller than the speed of sound in the material, and do well in describing the viscous regime. However, for materials under high stress this assumption must be re-examined for a more realistic calculation of the dislocation drag coefficient, including its velocity dependence. As a first step we study the velocity dependence in the subsonic regime, and intend to extend the theory to include dislocations moving at transonic and supersonic speeds in future work. The motivation for the latter comes from recent MD simulations and experiments which indicate the existence of dislocations moving at supersonic speeds — at least in certain materials such as plasma crystals [22], see also [18,23–29] and references therein.

In a previous paper [30], dislocation drag from phonon wind (from purely transverse phonons) was computed in the isotropic limit, mainly for simplicity, thereby generalizing the earlier models described in Ref. [9] to higher velocities. However, since the single crystal grains are typically a few microns up to a millimeter in size, dislocations travel in single crystals and occasionally cross boundaries, but never actually see an isotropic material. The purpose of the present paper is therefore to highlight the effect of crystal anisotropy on the dislocation drag coefficient from phonon wind by accounting for the crystal and slip plane geometries. As a first step towards a more sophisticated model, we keep the phonon spectrum isotropic for simplicity, but dislocations are modeled according to the crystal symmetry (bcc, fcc, hcp, etc.). We then compare to the purely isotropic results (now including also longitudinal phonons and thus generalizing [30]), seeing some deviations especially at high velocity, but even at small velocities for some materials. For the isotropic limit we use experimental polycrystalline elastic constant data. These deviations are expected since the present "semi-isotropic" approximation is able to capture features which are lost in the purely isotropic limit, such as the dislocation character dependence. Additionally the uncertainties in the experimental determination of elastic constants (both single and polycrystalline) — especially at third order — might also contribute to the deviations seen between the two methods for pure screw and edge dislocations at low velocity. In the high velocity regime, the observed large deviations between the two methods are expected since the position of divergences in the dislocation displacement gradient fields depends on the crystal geometry [31].

The outline of this paper is as follows: In Section 2 we start by reviewing the phonon wind contribution to the drag coefficient in the continuum approximation, following Ref. [30] for the purely transverse phonons, and subsequently generalizing to include also longitudinal phonons in Section 2.3. We then explain how to generalize the model to include anisotropic crystals, albeit assuming for simplicity an isotropic phonon spectrum. In Section 2.4 we then review the method of deriving the displacement gradient field of a dislocation moving at constant (sub-sonic) velocity and define the slip systems considered in the present case; see Refs. [31,32] and references therein for details. Finally, in Section 3 we present our results for dislocation drag in various metals of cubic, hexagonal, and tetragonal symmetry, and compare them to earlier experimental data, MD simulations, as well as our previous (more crude) purely isotropic model of [30], albeit now including also longitudinal phonons.

2. The phonon wind contribution to the drag coefficient

2.1. General considerations

In this work, we consider the harmonic approximation (where displacements are small compared to the lattice spacings) and take the continuum limit. We are interested in the interaction of phonons with a single moving dislocation in a crystal. Details of the derivation of the according Hamiltonian in the continuum description can be found in Ref. [30] — see also [9] and references therein for earlier work on this theory. Hence our starting point is the following Hamiltonian[2]:

$$\begin{aligned} &H = H_0 + H'(t)\,, \qquad H_0 = \textstyle\sum_{\vec{q}} \hbar\omega_q \left(\mathbf{a}_q^\dagger \mathbf{a}_q + \frac{1}{2}\right), \\ &H'(t) = \int_0^{2q_{\mathrm{BZ}}} \frac{dq\, q}{(2\pi)^2} \int_0^{2\pi} d\phi e^{-iqv|\cos\phi|\, t} \textstyle\sum_{\vec{q}} \Gamma_{q',q'-q}(q,\phi) \xi_{q'}^\dagger \xi_{q'-q}\,, \\ &\Gamma_{q'q''}(q,\phi) = \frac{\hbar}{4\rho\sqrt{\omega_{q'}\omega_{q''}}} \textstyle\sum_{i,j,k} d_{kk'}(q,\phi) \mathbf{w}_{q'i}^* \mathbf{w}_{q''j} \sum_{i'j'k'} q'_{i'} q''_{j'} \widetilde{A}_{ijk}^{i'j'k'}\,, \end{aligned} \tag{2.1}$$

consisting of the usual kinetic part for the phonons H_0 and the interaction between phonons and the dislocation H'. Following Ref. [9] we used the shorthand notation (or super-indices) $q' := \{\vec{q}, s'\}$; hence $\Gamma_{q'q''} := \Gamma_{s's''}(\vec{q}, \vec{q})$. Note that differences of super-indices mean the following: $\xi_{q'-q} := \xi_{\vec{q}-\vec{q},s'-s}$ and $\xi_{\vec{q},s} = \mathbf{a}_{\vec{q}s} + \mathbf{a}_{-\vec{q}s}^\dagger$. The phonon polarization vectors $\mathbf{w}_{qi} := \mathbf{w}_i(\vec{q}, s)$ satisfy the properties $\mathbf{w}_i(-\vec{q}, s) = \mathbf{w}_i^*(\vec{q}, s)$ and $\sum_i \mathbf{w}_i^*(\vec{q}, s)\mathbf{w}_i(\vec{q}, s') = \delta_{ss'}$ (orthonormality). The dimensionless phonon creation and annihilation operators satisfy the standard commutation relations

$$\left[\mathbf{a}_{\vec{q}s}, \mathbf{a}_{\vec{q}s'}^\dagger\right] = \delta_{\vec{q},\vec{q}}\delta_{ss'} \qquad \forall\, (\vec{q} - \vec{q}) \in \text{inverse lattice vectors}\,, \tag{2.2}$$

and all others vanishing. An important point to note here, is that we use, as an approximation, the isotropic Debye phonon spectrum using the effective Lamé constants of the polycrystal, i.e. "transverse" phonons are assumed to travel with a transverse sound speed computed from the effective polycrystalline shear modulus μ.

Our Hamiltonian (2.1) describes the interaction of phonons with (edge and screw) dislocations along the z-axis, moving with velocity v in the x-direction, and depending on the two-dimensional wave vector $\vec{q} = (q\cos\phi, q\sin\phi)$ of the dislocation. The field of displacement gradients due to the dislocation (in Fourier space) is denoted here by $d_{kk'}(q,\phi)$ and we will derive expressions for moving edge, screw, and mixed dislocations in Section 2.4. The phonon wave vectors $\vec{q}$, $\vec{q}$ lie in the first Brillouin zone and thus the dislocation wave vector satisfies $|\vec{q}| = |\vec{q} - \vec{q}| \le 2q_{\mathrm{BZ}}$ due to momentum conservation. For the edge of the Brillouin zone, we estimate q_{BZ} in such a way that it represents the radius of a sphere whose volume equals the unit cell volume in Fourier space, i.e. $q_{\mathrm{BZ}} = \sqrt[3]{6\pi^2/V_{\mathrm{c}}}$ where V_{c} denotes the volume of a unit cell.

Furthermore, ρ denotes the material density and the coefficients $\widetilde{A}_{ijk}^{i'j'k'}$ depend on second and third order elastic constants (SOEC and TOEC), $C_{ii'jj'}$ and $C_{ii'jj'kk'}$, via [33,34].

$$\widetilde{A}_{ijk}^{i'j'k'} = C_{ii'jj'kk'} + C_{ii'j'k'}\delta_{jk} + C_{jj'i'k'}\delta_{ik} + C_{i'j'kk'}\delta_{ij}\,. \tag{2.3}$$

The drag coefficient (or damping/friction "constant") B of a dislocation is defined as the proportionality coefficient of the force F needed to maintain dislocation velocity v. It is related to the dissipation D per unit length via $D = Bv^2$, which in turn is straightforwardly derived from the probability $W_{q'q''}$ of the scattering of a phonon from state q' to state q'' per unit time, see Refs. [14,17]. Multiplying $W_{q'q''}$ by the equilibrium phonon distribution function $n_{q'} = (\exp(\hbar\omega_{q'}/k_BT) - 1)^{-1}$ yields the number of transitions per unit time. Taking into account that an energy $\hbar(\omega_{q'} - \omega_{q''}) = \hbar\Omega_q$ is transferred for every transition, one finds for the dissipation per unit time and per unit dislocation length,

$$D = \frac{4\pi}{\hbar} \sum_{q',q''} \Omega_q\, |\Gamma_{q'q''}|^2 \left(n_{q''} - n_{q'}\right)\delta\left(\omega_{q'} - \omega_{q''} - \Omega_q\right), \tag{2.4}$$

where momentum conservation $\vec{q} = \vec{q} - \vec{q}$ is implicit so as to avoid clutter in the notation. The same expression can be derived from a one-

[2] Essential steps in deriving this expression are briefly outlined in Appendix A, albeit we refer the interested reader to Refs. [9,30] for further details.