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ORIGINAL PAPER

Modeling of Phonon Wind Shielding Effects on Moving Dislocation Arrays

A. M'ndange-Pfupfu · L. D. Marks

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Abstract An analytic geometric model of phonon–dislocation interaction is employed to simulate the shielding of phonon wind drag in moving dislocation arrays. In the model, we use assumptions that overestimate the shielding effect to calculate an upper bound for the deviation of drag on arrays from drag on single dislocations. For the system of a one-dimensional array of gliding dislocations in copper, we calculate that 6–25 % of the phonon drag is shielded by neighbor dislocations in the array. The model can be extended to other materials and dislocation distributions, but we show that for typical FCC crystals, calculating drag forces using a single dislocation is still a valid approximation.

Keywords Nanotribology · Friction mechanisms · Stress analysis

1 Background

As the scale of interest in materials design has become smaller, understanding the fundamentals of nanotribology has become more and more important. Not only do we need to understand and measure tribological properties but also we need to recognize the atomic-scale interactions that form the basis for friction and wear, so we can better control performance. Complicating this are scale-dependent changes in material behavior that often differ from the bulk, as well as new deformation mechanisms that may come into play at the nanoscale. Grain boundaries are one example of a nanoscale structure with significant implications for macroscale performance. Indeed, deformation by grain boundary rotation, recrystallization, and grain boundary sliding all play a role in the performance of crystalline materials. Modeling these phenomena is therefore an important part of our overall understanding.

Dislocations have long been used as a framework for understanding crystalline materials, particularly under applied stress. It has been found that the properties and interactions of dislocations have a significant effect on macroscale behavior, and dislocation theory has well-established predictive power. This dislocation framework can be extended beyond plastic deformation to include the modeling of more general friction and wear phenomena, which can give us new tools and insights useful for analyzing complicated tribological systems [1–3]. We have shown that it is feasible to express friction at a crystalline interface in terms of misfit dislocation drag [4], and that plowing friction in certain temperature–pressure regimes can be associated with power-law dislocation creep [5]. In both of these cases, and dislocation theory in general, the forces on a single dislocation are considered. In this article, we want to consider more closely the motion of an array of dislocations.

Stable arrays of dislocations form when nearby dislocations are attracted into an energy-lowering configuration. Many such equilibrium distributions of dislocations are possible, including tilt and twist boundaries, but non-equilibrium configurations are also seen, for instance, Read and Shockley [6] showed that any low-angle grain boundary can be thought of as an array of dislocations. Arrays of dislocations are therefore involved in material deformation, in an accommodating way such as glide on a slip plane or grain boundary rotation [7–10], or as barriers

A. M'ndange-Pfupfu (✉) · L. D. Marks
Department of Materials Science and Engineering, Northwestern University, 2220 N. Campus Drive, Cook Hall Room 2036, Evanston, IL 60208, USA
e-mail: ariel@u.northwestern.edu

such as in the cases of dislocation pile-up [11–13]. The motion of such arrays is therefore important to understand the deformation, and by extension, the tribological behavior of the crystal. We concentrate here on the effects of phonons on that motion.

The viscous interaction between phonons and the stress fields of dislocations is well understood and a significant contributor to the drag force on moving dislocations in crystalline solids [14–17]. Phonons can be generally thought of as elastic waves with a frequency and energy, with a density of states throughout k-space. Like other collective oscillations, phonons can be considered quasi-particles carrying a pseudomomentum $\hbar k$, where k is the reciprocal lattice vectors and $\hbar$ is Planck's constant. When they fall within the appropriate energy range, phonons can be scattered inelastically by dislocations. During a scattering event, a phonon can transfer part of its momentum to a dislocation; therefore, a moving dislocation will encounter a net loss in momentum in a viscous manner, due to the anisotropy of incident phonons. Particularly at low temperatures where thermally activated dissipation mechanisms are limited, this phonon wind effect can be an important component of dislocation drag, and by extension, frictional losses.

Like other forms of macroscale viscous drag, we hypothesize that the drag force due to the phonon wind should be partially shielded when incident on a moving array of dislocations. In particular, first-order shielding effects should cause the array as a whole to experience proportionally less drag than a single dislocation in isolation. We use a geometric model to estimate the magnitude of the shielding effects and determine the validity of the ubiquitous single-dislocation approximation.

2 Model

We consider a one-dimensional array of dislocations in copper gliding on a slip plane, as shown in Fig. 1a. The amount of shielding is geometrically determined, and depends on the scattering cross-section r of a dislocation to an incident phonon wavetrain, as well as the spacing s between dislocations.

We consider the dislocations in two dimensions as circles with radius equal to the scattering cross-section for the phonon scattering interaction. We assume that phonon scattering events prevent 100 % of the phonon momentum from being transmitted farther along that vector.

The greatest amount of shielding will be from the nearest neighbor, so we can consider a two-dislocation system as shown in Fig. 1b. From the coordinate system of a dislocation, we consider incident phonons that have a component coming from the direction of motion $\vec{v}$ in the figure. That is to say, we take into account all phonons incident between $\theta = -90°$ and 90°, as measured from the vertical. We consider the angles shielded α at each angle θ on the forward-facing half-circle of the dislocation. Taking the ratio of the shielded to unshielded angles, we integrate to yield the amount of phonon momentum shielded as a percentage of the total momentum.

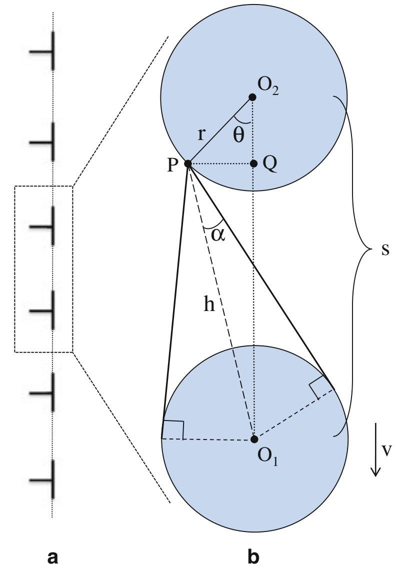

Fig. 1 **a** A typical array of edge dislocations with the same Burgers vector glide through a crystal on a slip plane. We consider phonons incident on the array with momentum counter the direction of motion. **b** Nearest neighbor dislocations in a 1D array are represented as *spheres*, and reduced here to *circles* due to spherical symmetry. Their spacing is s, their scattering cross-section is r, and they move with velocity v. At every point P on the forward-facing half-circle of the shielded dislocation O_2, the angles shielded due to O_1 are calculated using h and θ and integrated to yield the total percentage of the half-circle shielded

Let us first consider the right triangle with hypotenuse h formed by points O_1, P, and Q. The horizontal and vertical sides can be calculated using the trigonometry of the circle O_2. We then use the Pythagorean Theorem and simplify:

$$h = \sqrt{(r\sin\theta)^2 + (s - r\cos\theta)^2} = \sqrt{r^2 + s^2 - 2sr\cos\theta}. \quad (1)$$

Next, we look at the right triangle formed by O_1, P, and a tangent point to circle O_1. Again the hypotenuse is h, so we can write the equation for α by rearranging the trigonometric relationship:

$$h\sin\alpha = r$$
$$2\alpha = 2\sin^{-1}\left(\frac{r}{h}\right).$$

Finally, we integrate over the edge of the shielded dislocation. The occluded portion of the half-circle, integrating over θ, is given by:

$$2\int_0^{\frac{\pi}{2}} \frac{2\alpha}{\pi} d\theta.$$

We subtract this from the total integral over the half-circle, and using (1) this yields the proportion of incident phonon momentum exposed to the shielded dislocation (2).

$$2\int_0^{\frac{\pi}{2}} 1 d\theta - 2\int_0^{\frac{\pi}{2}} \frac{2\alpha}{\pi} d\theta$$
$$= \pi - \frac{4}{\pi}\int_0^{\frac{\pi}{2}} \sin^{-1}\left(\frac{r}{\sqrt{r^2 + s^2 - 2sr\cos\theta}}\right) d\theta. \quad (2)$$

We take the dislocation Burgers vector b as that of a typical FCC metal slip plane, and use a range of 2.5–2.88 Å, encompassing copper, aluminum, nickel, silver, gold, and platinum [18, 19]. The relevant scattering cross-section is taken to be twice the Burgers vector as suggested by Hikata et al. [20]. The scattering cross-section is also dependent on the incident phonon angle, and for random incident angles the adjustment to r can be calculated to be between 0.5 and 2 times [21]. Results are presented for a variety of dislocation spacings, as this will be determined by the experiment.

When considering the incident phonon momentum, we realize that the contribution to the drag force (in Fig. 1b, the vertical component in the $-v$ direction) depends on the cosine of the angle between the phonon wavetrain and the dislocation motion—in our system, this adds a factor of $\cos\theta$. For a typical shielding of 15° around the vertical, however, the contribution to the drag from shielded dislocations is >96 %, and in the model we consider the contribution to be 100 %, which is a slight overestimate.

3 Results and Discussion

Figure 2 shows the phonon exposure of the shielded dislocation as a percentage of the full unshielded exposure, calculated numerically from (2).

Under these conditions we see that for $r = 2b$, the exposure is 88 % at the closest geometrically possible spacing.

The model shows the effect of shielding as a function of scattering cross-section and dislocation spacing. If we consider that in actual materials, phonon momentum will not be completely absorbed by the first interaction, we can see that unsurprisingly, we are left with a negligible effect in most situations. Throughout our calculations, we considered the maximum possible drag reduction, and were still left with a small effect. This is consistent with the typical experimental result that matches single-dislocation theory within 10–15 %.

The three-dimensional symmetry of our system means the proportional reduction in drag is the same as the two-dimensional result, when all dislocations have the same length. However, the model could be extended to take into account more complicated arrays of dislocations in more than two dimensions. However, because of the previously mentioned diminishing component of shielded momentum

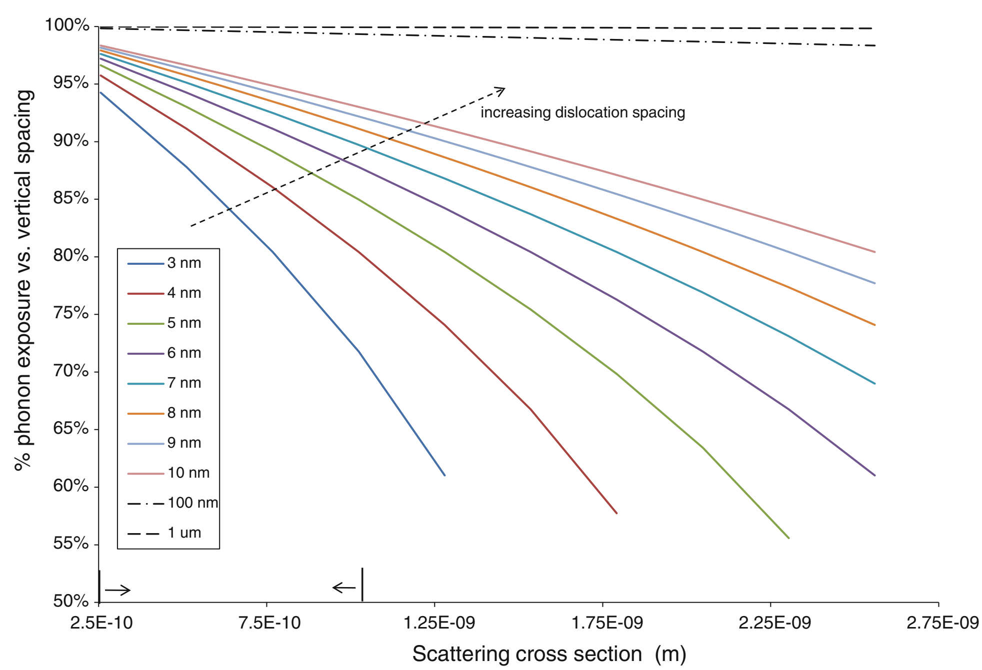

Fig. 2 The percentage of phonons that will be incident on the shielded dislocation, as a function of scattering cross-section—100 % represents no shielding effect, 0 % represents complete shielding. Results for a range of spacings are shown. The relevant cross-sections are indicated with bounding *arrows*, encompassing the range between one-half and twice the average $\sigma = 2b$

in the drag direction with higher angles θ, the nearest neighbor dislocation in the direction of motion—as we have considered–will be the dominant scatterer.

It is important to remember that phonons are collective oscillations of the entire crystal lattice and therefore a long-range phenomenon. Local disruptions in the strain field, such as point defects, would not be expected to affect an array of dislocations any differently than a single dislocation.

4 Conclusion

We use a geometric model to account for the shielding effect of nearest neighbors on the phonon wind drag experienced by moving dislocations in a one-dimensional array. We consider the case where scattering events shield 100 % of the phonon momentum, to calculate the theoretical maximum reduction in drag due to this effect. As expected, even with our assumptions creating an overestimate of the true effect, the shielding effect is relatively small. For the relevant scattering cross-section for copper, we can calculate the reduction in phonon momentum incident on shielded dislocations as not exceeding 12 %, the shielded portion of the half-circle at the closest spacing. Considering the variability in the scattering cross-section, we conclude that treating an array of moving dislocations as a single dislocation results in an overestimate of at most 6–25 %, which can be considered valid. Although dislocation arrays remain important structures with distinct properties, our modeling shows that shielding effects are not a significant factor in their drag behavior.

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