AMPLITUDE DEPENDENT INTERNAL FRICTION WITHIN A CONTINUUM SIMULATION

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ABSTRACT

The mechanical losses due to the bowing of isolated Frank-Read sources under application of periodic loads is studied within a continuum simulation of dislocation dynamics. The dislocations are modelled within isotropic elasticity theory and assumed to be in the overdamped limit. Dislocation radiation effects are neglected. The mechanical losses are studied as a function of bias stress, amplitude of the periodic stress and frequency. The frequencies studied lie between 10 KHz and 1 MHz. Under high stresses applied at low frequencies, a deviation from the expected Lorentzian resonance shape is observed. The physical origins of this deviation are discussed.

INTRODUCTION

The motion of dislocations under periodic loads is known to contribute to losses measured during internal friction experiments [1]. Therefore, under ideal circumstances, internal friction experiments offer a means to explore the dynamics of dislocations. For example, in materials with a large Peierls barrier, one may deduce the dislocation kink pair formation energy [2].

However, other microscopic mechanisms, for example atomic scale diffusion, may lead to mechanical losses. Proper interpretation of internal friction experiments, therefore, requires a detailed theory-based understanding of the phenomenon in question. Identifying the proper theory, then, is a central to efforts aimed at advancing applications of mechanical spectroscopy techniques for studies of dislocation dynamics.

For describing materials with a small Peierls barrier, such as aluminium, the model most often applied is that of a vibrating string, explored originally within this context by Granato and Lücke [3]. A straight elastic string is pinned at both ends, the resonant frequencies of the string are calculated, and the losses associated with the resonances summed to yield a final expression for the total loss. Implicit in this model is the assumption that the displacement of the string is small in comparison to its length, and that the amplitudes of any residual or bias stresses are zero.

To address the large stress amplitude regime, Tyapunina and Blagoveshchenskii[4] applied a numerical approach to study large displacements of an elastic string governed by viscous dynamics. They demonstrated that the internal friction expected from a bowing Frank-Read source displays both frequency and stress amplitude dependences. However, their approach assumed a constant, isotropic line tension, and hence did not represent fully the change in dislocation self stress with the configuration of the dislocation. Further, their work did not consider the effects of a static bias stress on the expected loss.

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In the current work, simulations of dislocation dynamics are used to explore the mechanical losses expected from the simultaneous application of static and periodic loads to a Frank-Read source. The losses are studied as a function of periodic stress amplitude, bias stress and frequency. The results are compared with the expectations of the Granato-Lücke formalism. In particular, it is noted that under common circumstances one may observe significant deviations from the form expected based on the elastic string model.

MODEL

The dislocations are assumed to be governed by isotropic elasticity theory and embedded in an infinite and homogeneous medium. The dynamics are assumed overdamped, so that the dislocation mass may be neglected. The drag coefficient is assumed independent of velocity and isotropic with respect to the orientation of the dislocation.

A previously developed simulation code [5] incorporating these features is applied to calculate the dynamic response of the dislocations. The simulations treat the dislocations within a continuum limit, and reflect the full self-stress of the dislocations. Elastic parameters consistent with Aluminium, *i.e.*with the magnitude of the Burgers vector $b = 2.86$ Å , the shear modulus is taken to be $\mu = 26.5$ GPa, and the drag coefficient is taken as $B = 0.08$ N s m^{-2}. The dislocation is treated as if undissociated. The small scale cutoff procedure employed by Hirth and Lothe [6] is applied, and the cutoff is chosen to be $\rho = 10$ Å.

The dislocation is decomposed into segments extending between points. The points are indexed by the subscript i and the vector $\hat{\mathbf{u}}_i$ indicates the glide direction normal to the dislocation line direction at point i. The velocity of the ith point is given by

$$\frac{\partial \mathbf{u}_i}{\partial t} = \frac{(((\boldsymbol{\sigma}_i \cdot \mathbf{b}) \times \boldsymbol{\xi}_i) \cdot \hat{\mathbf{u}}_i)\, \hat{\mathbf{u}}_i}{B}. \tag{1}$$

Where $\boldsymbol{\xi}_i$ and $\boldsymbol{\sigma}_i$ are the line direction and stress at the ith point, $\mathbf{b}$ is the burgers vector. The stress $\boldsymbol{\sigma}_i$ reflects the contributions from the applied stress as well as the self-stresses of the dislocation. Radiated elastic waves are not considered.

Eqs. (1) are integrated using a fourth order Runge-Kutta integration scheme, as outlined in reference [5], with the exception that additional points are now inserted along a fitted spline, instead of inserting points along a fitted circle.

SIMULATIONS

The simulations consider dislocation configurations similar to that shown in Fig. 1. The losses associated with the application of the periodic stress are calculated as follows. The periodic and bias stresses are applied to the dislocation, and the hysteresis is recorded. The simulations are run until "steady-state" hysteresis is observed. This condition is defined practically as the point at which the area swept out over a complete cycle remains fixed from cycle to cycle (within the noise limits of the simulations). Once "steady-state" is attained, the hysteresis is averaged over eight cycles and the energy loss from the dislocation is calculated according to

$$\Delta W \propto \left\langle \int_{\tau}^{\tau+2\pi/\omega} \sigma_a(t) d\varepsilon \right\rangle \propto \left\langle \int_{\tau}^{\tau+2\pi/\omega} \sigma_\omega \cos(\omega t) b \frac{\partial A}{\partial t} dt \right\rangle, \tag{2}$$

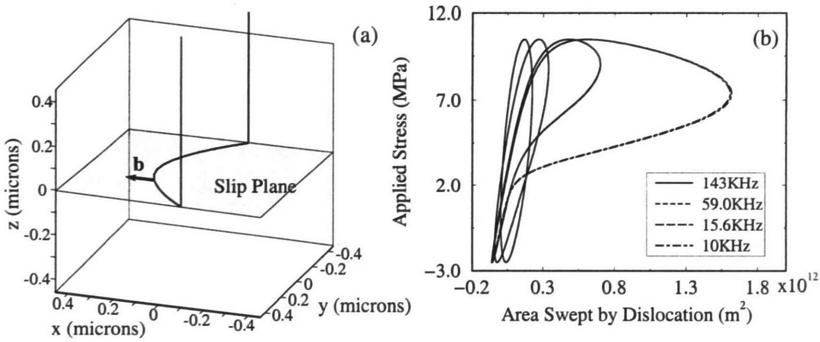

Figure 1: (a) A typical configuration of the Frank-Read Sources. Note that the arms carry on out of the diagram and the loop is closed on a parallel plane 10 μm above the slip plane. (b) The evolution of the hysteresis loop as the frequency drops through the peak loss frequency for a 1 μm edge oriented source $\sigma_{bias} = 4$ MPa and $\sigma_\omega = 6.5$ MPa.

where τ is a time in the "steady state" regime, ω is the angular frequency, and $\sigma_a(t)$ is the applied stress at time t. The time dependent strain from the motion of this dislocation, ε, is taken to be proportional to $A(t)$, the area swept out by the dislocation at time t. In short, ΔW is taken to be proportional to the area of the hysteresis loop (Fig. 1). The applied stress is given by $\sigma_a(t) = \sigma_{bias} + \sigma_\omega \cos \omega t$ with σ_{bias} a static applied stress, and σ_ω the amplitude of the periodic component of the stress. The simulations are run at a number of angular driving frequencies in the range from 10KHz to 1MHz. A peak is seen in the energy absorption as function of frequency. This absorption peak is studied for a variety of different stress conditions for both screw and edge dislocation sources of varying lengths. Typical results are depicted in Fig. 2.

DISCUSSION

The data in Fig. 2 represent the losses calculated from a 1 μm length source. For low bias stresses and high frequencies, the peak resembles the Lorentzian shape expected from a 1-dimensional linear, overdamped oscillator:

$$\Delta W = \frac{\omega D \sigma_\omega^2}{k^2 + (\omega D)^2}. \tag{3}$$

Here, D is a drag coefficient for the oscillator, and k represents the spring constant. From the form of Eq. (3), it is apparent that if one increases the value of k, the peak is shifted to higher frequencies, and the maximum loss is reduced. Increasing the drag coefficient D simply translates the entire curve to lower frequencies. Eq. (3) thus serves as a simple model for the losses observed in the more complicated dislocation problem, and the features evident in Fig. 2 are discussed in terms of the parameters k and D.

stiffness vs. length

Panel (b) of Fig. 3 displays a scaled plot of the area of a dislocation loop vs. the applied, subcritical stress. One expects this area to scale as L^2, where L is the length of the source.

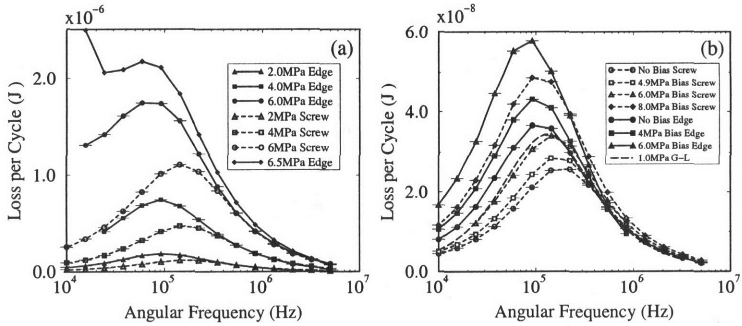

Figure 2: The mechanical loss from 1μm edge and screw sources (a) under 4 MPa bias stresses with differing σ_ω, and (b) with $\sigma_\omega = 1$ MPa for the indicated values of σ_{bias}. Panel (b) also shows the loss predicted from Granato-Lücke theory. Note that the predictions of Granato-Lücke and the current theory are similar when $\sigma_{bias} = 0$ and for low values of σ_ω.

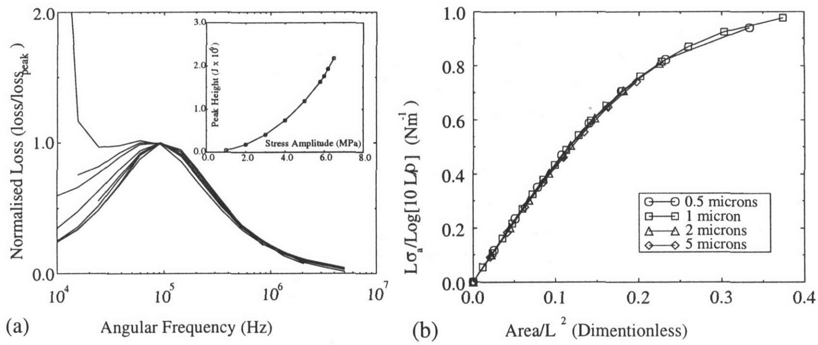

Figure 3: (a) The normalized loss for 4.0 MPa biased, 1μm edge sources subject to different driving stresses with the change in peak. Loss with stress amplitude shown inset. (b) The scaled stress-area curve for quasi-static bowing of different length edge sources.

Similarly, one expects that the critical stress to set the relevant stress scale. The critical stress scales as $(L/\log CL)^{-1}$ with C a constant. Fitting to the results of reference [5] one finds that $C \approx 1.6 \times 10^9$. The implication is that one might scale the stress axis by the factor $L/\log\frac{1.6L}{\rho}$ and the area axis by a factor of L^{-2} and produce one scaled plot of applied stress as a function of area swept out. It turns out that better data collapse is obtained for the choice $C = 10/\rho$. The plot so obtained is contained in panel (b) of Fig. 3. The data collapse is excellent, though the precise origin of the value of C which gives the collapse is not well understood.

The slope of the stress vs. area curve, then, represents the area dependent stiffness, k. It is apparent that at higher scaled stresses, the stiffness of the loops is reduced, and eventually, near a scaled stress of 1, the stiffness becomes identically zero.

edge vs screw

Fig. 2 indicates that the losses associated with initially screw oriented segments are lower than their edge oriented counterparts. This is a consequence of the elastic strain energy difference between the screw and edge segments. The elastic strain energy of a screw dislocation is reduced relative to the edge dislocation by a factor of $1 - \nu$. Hence bowing the screw dislocation, so that part of it assumes edge character, requires more stress than bowing the edge segment to a partial screw orientation. The net result is that for the screw oriented segments, the effective value of k is larger.

stress amplitude

Fig. 2 also indicates that as the amplitude of the periodic stress is increased, the magnitude of the loss increases as well. One expects the losses to scale with the square of the periodic stress amplitude, and this behavior is observed (Fig. 3). The shift in peak frequency with increasing amplitude apparent in Fig. 2 stems from the softening of the dislocation line tension as the dislocation bows. The effective stiffness, k is thus amplitude dependent.

bias stress

For large bias stresses, the form of the loss curve can differ dramatically from the simple Lorentzian shape (Figs. 2 and 3). Specifically, the loss reveals a rapid rise at low frequencies. The physical origins of this rise are clear. Consider the situation in which the sum of σ_ω and σ_{bias} exceeds the critical stress necessary to operate the Frank-Read source. Then, as $\omega \to 0$, the dislocation behaves as an overstressed source. Earlier work has demonstrated that there is a stress dependent characteristic time to operate a Frank-Read source, and that this time increases rapidly as the critical stress is approached from above [5]. Then, the reciprocal of this characteristic time sets a characteristic frequency for losses during internal friction. Frequencies much higher than this characteristic frequency will yield small losses. As the characteristic frequency is approached from above, the losses will begin to increase as the dislocation is moved back and forth through the critical configuration. At even lower frequencies, the loss per cycle is not constant, as the dislocation motion is no longer periodic.

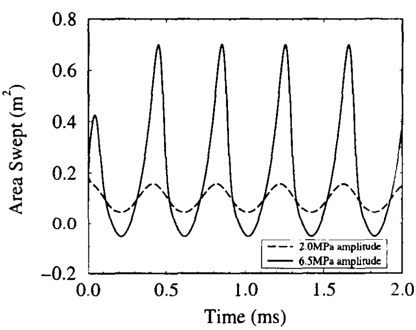

Figure 4: Area vs. time curves for $\sigma_\omega = 2.0$ MPa (dashed line) and $\sigma_\omega = 6.5$ MPa (solid line) with $\sigma_{bias} = 4.0$ MPa. The large amplitude area shows marked deviations from a simple cosine form.

Within the model summarized in Eq. (3), the picture is as follows. For high frequencies, the displacement due to the periodic stress is small, and the stiffness of the dislocation is determined by the local slope of the stress vs. area curve shown in Fig. 3. However, as the amplitude of the periodic stress is increased, the effective stiffness of the dislocation can be driven towards the value zero, as the dislocation oscillates about the maximum shown in panel (b) of Fig. 3. This leads to the rise in losses at low frequencies. Based on this simple argument, one would expect to observe larger shifts in the peak frequency than those observed. This lack of large shift is explained as an overall decrease in the effective drag coefficient D which partially cancels the shift arising from the decrease in stiffness.

The effects of the σ_{bias} and σ_{ω} are readily observable in plots of area swept out vs. time for the driven dislocation. Fig. 4 displays two area vs. time curves, one for a large amplitude oscillatory stress, and a second for a small amplitude. The small amplitude curve is described well by a simple cosine. The large amplitude curve, in contrast, shows large deviations from the simple cosine form.

CONCLUSIONS

In conclusion, dislocation dynamics simulations are used to investigate the amplitude and bias stress dependence of losses due to oscillating dislocations. A simple overdamped oscillator model is used characterize the response of the dislocation to time dependent loads. The amplitude dependence of the losses scales roughly as the amplitude of the oscillatory component of the stress squared. The results are found to be in good agreement with expectations based on the theory of Granato and Lücke for the range of stresses in which that theory is likely to apply.

A striking feature of the losses is their frequency dependence. For large frequencies and small bias stresses, the frequency dependence displays a single peak. However, for larger bias stresses, and lower frequencies, the loss spectrum includes the expected peak, but also reveals a divergence at lower frequencies. This divergence arises from the fact that the effective stiffness goes to zero near the critical stress for operation of a Frank-Read source.

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REFERENCES

1. G. Fantozzi, C. Esnouf, W. Benoit and I. G. Ritchie, *Prog. Materials Sci.* **27**, 311 (1982).

2. A. Seeger, *Phil. Mag.* **1**, 651 (1956).

3. A. Granato and K. Lücke, *J. Appl. Phys.* **27**, 583 (1956).

4. N. A. Tyapunina and V. V. Blagoveshchenskii, *Phys. stat. sol.(a)* **69**, 77 (1982).

5. A. K. Faradjian, L. H. Friedman and D. C. Chrzan, *Modelling Simul. Mater. Sci. Eng.* **7**, 479 (1999).

6. J. P. Hirth and J. Lothe, *Theory of Dislocations*, Krieger Publishing Company, Malabar, Florida, second ed. (1992).