Mechanical Damping due to Interfacial Motion in Micro-Resonators

D.N. Pawaskar and R. Phillips

Department of Mechanical Engineering
California Institute of Technology
Pasadena, CA 91125
{pawaskar,rphil}@caltech.edu

ABSTRACT

Mechanical damping influences the sensitivity and resolution of micro sensors and actuators. In this paper, we have investigated one of the mechanisms responsible for dissipation of vibrational energy, namely motion of grain boundaries. The focus has been on modeling the movement of the grain boundary perpendicular to the interfacial plane. To this end, we have modeled the interface as an array of dislocations. By accounting for all forces acting on individual dislocations, we are able to extract the effective motion of the interface and thus compute cyclical energy losses. We have computed the dependence of the mechanical quality factor on the grain boundary misorientation and its geometric inclination with respect to the vibrating beam.

Keywords: damping, dissipation, energy, micro, oscillators

1 INTRODUCTION

Oscillators with characteristic dimensions in micro/nano meters have been finding increasing uses as sensors and actuators. Typical examples of such applications include probes for measurement of force, displacement, and acceleration [1]. One of the principal dynamic properties of such systems is the quality factor, Q defined to be,

$$Q = 2\pi \frac{E_m}{E_d} \tag{1}$$

where E_m is the maximum mechanical energy in the system and E_d is the energy dissipated in one cycle of oscillation. Thus, Q, is a measure of vibrational damping in the system. One of the principal advantages in employing small system sizes is that the sensitivity and resolution of the transducer can be boosted by Q. In particular, an elementary spectral analysis shows that sensitivity $\sim Q$ and the resolution $\sim \sqrt{Q}$. The various possible mechanisms responsible for lowering the Q of an oscillator are: damping due to the surrounding fluid, losses due to mechanical energy being leaked away to an elastic support, energy dissipation due to the inherent thermoelasticity of the beam material, surface effects such as structural rearrangements, and losses due to internal friction caused by the motion of lattice defects [2].

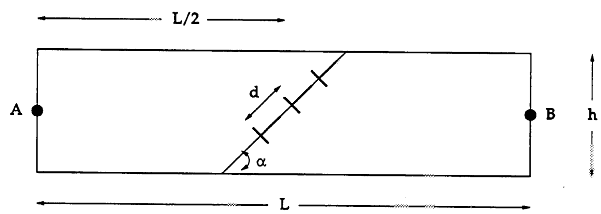

Figure 1: Setup under consideration showing a low angle grain boundary in a simply supported beam of length L approximated by an array of dislocations with an inter-dislocation spacing of d. h is the height of the beam. A and B are pin supports.

In this paper, we have investigated grain boundaries as possible agents for intrinsic losses in micron level oscillators. This has been done with a view to establishing a connection between macroscopic system dynamics and microstructural features of a model device.

2 MODELING AND SIMULATION

The prototypical oscillator is the one showed in fig.1. It consists of an aluminum beam of length 1μm, pinned at its ends. A low-angle tilt grain boundary is built into the beam as shown such that the midpoint of the boundary coincides with the centroid of the beam. The height and width of the beam are both 0.1μm. A low-angle tilt grain boundary can be considered as an array of edge dislocations. The small misorientation angle can then be obtained as $b = d\theta$ where d is the inter-dislocation spacing and b is the Burger's vector of the dislocation. The power of the dislocation-based model lies in the fact that we can model the physics of the interface based completely on the mechanics of its constituent dislocations. The combined motion of all the dislocations can be said to be the effective motion of the interface. The equation of motion for a dislocation is,

$$B\dot{x} = f = (\bar{\sigma}_{ij} + \hat{\sigma}_{ij} + \sum \tilde{\sigma}_{ij}) b_i n_j \tag{2}$$

where f is the Peach-Koehler force due to all applied stresses in the body and we have neglected inertial effects. These stresses are $\bar{\sigma}$, the oscillating applied stress due to beam bending, $\hat{\sigma}$ the image stresses that arise because of the presence of free surfaces, and $\tilde{\sigma}$ the interaction with all other dislocations. The Peierls' stress of an edge dislocation in aluminum is very small and hence negligible [3]. Now eq. (2) can be rewritten as,

$$Bv + (K_s + K_d)x = f_b \sin \omega t \tag{3}$$

where f_b is the amplitude of the time-dependent Peach-Koehler force and $K_s x$ and $K_d x$ refer to the surface and inter-dislocation interactions respectively, which depend linearly on small excursions of the dislocation from its mean position. The quantity $K_s + K_d$ is thus the effective stiffness of the grain boundary. It has two contributions, one from the inter-dislocation interaction and the other from the free surfaces that surround the grain boundary. We now present a detailed computation of each of terms in this equation.

1. Bending Stress

For the sake of analytical tractability, we consider all dislocations to be situated on the grain boundary line itself. We invoke Euler-Bernoulli beam theory to calculate the bending stress at any point (x, y) in the beam according to $\bar{\sigma} = yEU_{xx}$. Now we assume that the beam is vibrating in its mth mode of vibration. In this case, the displacement of the beam is given by $U(x,t) = U_0 \sin \omega t \sin \frac{m\pi}{L} x$ where U_0 is the amplitude of vibration supplied as an initial condition. In keeping with the assumptions of Euler-Bernoulli beam theory, we will work with small amplitudes, i.e. $U_0/L \approx 0.05$. The bending stress gives rise to a Peach-Koehler force which acts on every individual dislocation. The glide component of this force which is responsible for the motion of the dislocations in their own slip planes, is given by $f_b = \bar{\sigma}_{ij} b_i n_j$. The normal to the slip dislocation plane is $\mathbf{n} = (\cos\alpha, \sin\alpha)$ and the Burger's vector is $\mathbf{b} = b(\sin\alpha, -\cos\alpha)$. We use this to obtain,

$$f_b = \frac{1}{2} E y U_0 b \sin 2\alpha (\frac{m\pi}{L})^2 \sin \frac{m\pi}{L} x. \tag{4}$$

Now since every dislocation in the beam can be geometrically located through $x = L/2 + d\cos\alpha$ and $y = d\sin\alpha$, eq. (4) will provide the harmonic force due to free vibrations of the beam on every dislocation. Note that this is an external force from the perspective of the dislocations.

2. Viscous Damping

The resistive force on a moving dislocation, called dislocation drag, depends on many factors. Theoretical treatments [4] show conclusively that the drag force caused by such mechanisms is directly proportional to the dislocation velocity, v. This viscous damping behavior is expressed by,

$$f_{drag} = Bv \tag{5}$$

where B is the constant of proportionality called the drag constant or drag coefficient. We use 10^{-4} Pa s as the dislocation drag coefficient at room temperature in accordance with the works of [5].

3. Elastic Interactions

These effects include: dislocation-dislocation interactions and dislocation-surface interactions.

3.1. Inter-Dislocation Interactions

The force on any dislocation is obtained by summing over its interactions with all N dislocations. The total number of dislocations N is obtained from geometric considerations. Refer to fig.1. We assume that all dislocations are evenly spaced along the grain boundary. Then,

$$N = \text{nint}(\frac{h\theta}{b \sin\alpha}) + 1 \tag{6}$$

where we have used $b = d\theta$ and $\text{nint}(r)$ yields the nearest integer to the real number r. N is thus the total number of degrees of freedom in the dislocation dynamics simulation. Now consider the two edge dislocations m and n located at (x_m, y_m) and (x_n, y_n) respectively. The slip planes of the two dislocations are parallel to each other and their Burgers' vectors point in the same direction. d is the distance between the slip planes of two consecutive dislocations. Let us write $x = x_n - x_m$ and $y = y_n - y_m = (n-m)d$. Assuming that dislocation m is stationary, the Peach-Koehler force per line length on dislocation n is given by $f_{mn} = \bar{\sigma}_{xy}^{(m)} b^{(n)}$ Substituting $\sigma_{xy} = Ax\frac{x^2-y^2}{(x^2+y^2)^2}$ [6] where $A = \mu b / 2\pi(1-\nu)$ we get the total force exerted on one dislocation n due to all other dislocations. Assuming small displacements, the elastic stiffness arising out of interdislocation interactions works out to,

$$K_d^{(n)} = \frac{\mu b^2}{2\pi(1-\nu)d^2} \sum_{m \neq n}^{m=N} \frac{1}{(n-m)^2} \tag{7}$$

Eq. (7) is a ready recipe for computing this stiffness for every dislocation in the array. We now proceed to obtain a similar elastic stiffness due to the effect of free surfaces that surround the grain boundary in the beam.

3.2. Surface Effects

A free surface attracts dislocations and other crystal defects in an attempt to minimize the total potential energy of the system. The surface force on a dislocation is the Peach Koehler force exerted by its image. In general, it is very difficult to analytically calculate the surface forces experienced by an arbitrarily inclined dislocation. Hence we have to resort to numerical techniques to solve this problem. The finite element method has

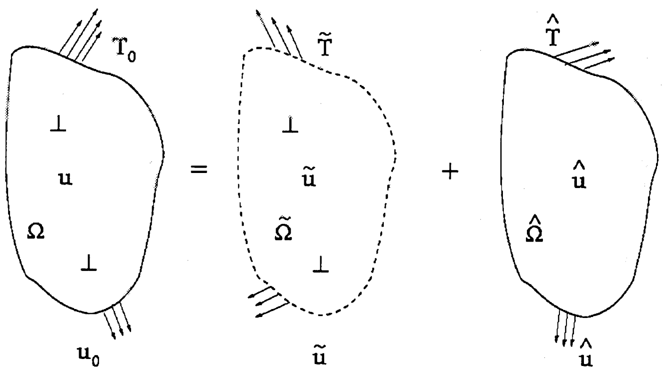

Figure 2: Schematic of computing elastic fields in a finite body containing discrete dislocations by the finite element method. Source: van der Giessen and Needleman (1995).

been extensively used to simulate the behavior of discrete dislocations in a finite body. Fig. 2 is a schematic illustrating the method of computing surface forces on dislocations in a finite solid. This procedure is based on the discrete dislocation modeling techniques used by [7]. Let $\mathbb{E}$ represent the set of elastic fields, namely stresses, strains, and displacements $\{\boldsymbol{\sigma}, \boldsymbol{\epsilon}, \mathbf{u}\}$. The elastic fields in a finite body (Ω) on the left can be split by linear superposition into two additive components.

$$\mathbf{u} = \tilde{\mathbf{u}} + \hat{\mathbf{u}}, \qquad \boldsymbol{\epsilon} = \tilde{\boldsymbol{\epsilon}} + \hat{\boldsymbol{\epsilon}}, \qquad \boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \hat{\boldsymbol{\sigma}}. \qquad (8)$$

The ($\widetilde{\mathbb{E}}$) fields are associated with N dislocations in their current configuration in an infinite body with elastic modulus tensor $\mathbf{C}$, based on Volterra's solution [6]. These fields are obtained by superposing all the fields of the individual dislocations, These fields are governed by the standard equations of linear elasticity in the region $\widetilde{\Omega}$ which are,

$$\nabla \cdot \tilde{\boldsymbol{\sigma}} = \mathbf{0}, \qquad \tilde{\epsilon} = \text{symm}\nabla\tilde{\mathbf{u}}, \qquad \tilde{\boldsymbol{\sigma}} = \mathbf{C} : \tilde{\epsilon}. \qquad (9)$$

This results in boundary tractions and displacements on the fictitious boundary $\partial\widetilde{\Omega}$.

$$\tilde{\boldsymbol{\sigma}}\mathbf{n} = \tilde{\mathbf{T}}, \qquad \mathbf{u} = \tilde{\mathbf{U}}. \qquad (10)$$

The $\widetilde{\mathbb{E}}$ fields are easily obtained since there is no boundary in their domain over which they apply. But now it becomes necessary to recover the actual boundary conditions on Ω which we managed to disturb through the $\widetilde{\mathbb{E}}$ fields. This is achieved through the correction $\widehat{\mathbb{E}}$ fields in the domain $\widehat{\Omega}$. The boundary value problem to be thus solved is formulated as follows. In $\widehat{\Omega}$, eq. (9) holds for the $\widehat{\mathbb{E}}$ fields. Over the boundary $\partial\widehat{\Omega}$

$$\hat{\boldsymbol{\sigma}}\mathbf{n} = \mathbf{T}_0 - \tilde{\mathbf{T}}, \qquad \hat{\mathbf{u}} = \mathbf{u}_0 - \tilde{\mathbf{U}}. \qquad (11)$$

We have implemented a finite element solution of this problem in ABAQUS, a commercial finite element program. Thus, the surface force on a dislocation is the Peach-Kohler force due to the residual stress field $\hat{\boldsymbol{\sigma}}$ on the dislocation, $f_s = \hat{\sigma}_{ij} b_i n_j$. To calculate the surface stiffness, we calculate the slope of the surface force-displacement curve for each of the N dislocations in the beam by slightly perturbing every dislocation away from its equilibrium position.

4. Dislocation Dynamics

For a particular dislocation n , eq. (2) is rewritten in a discrete form suited for computations as an $N \times N$ system,

$$B\dot{x} + Kx = f \qquad (12)$$

This system is numerically solved by exciting the beam in a particular mode and amplitude so that the frequency and forcing is available. Then the system is evolved in time which results in the displacement $x_n(t)$ of each dislocation in the system. The dissipation in one cycle is then given by

$$E_d = \sum_{n=1}^{N} \int_0^{\frac{2\pi}{\omega}} B\dot{x}_n(t) \cdot \dot{x}_n(t) \mathrm{d}t. \qquad (13)$$

The quality factor is given by eq. (1) where E_m is

$$E_m = \frac{1}{2} EI \int_0^L U_{xx}^2 \mathrm{d}x. \qquad (14)$$

The time integration of eq. (12) has been implemented in MATLAB. where in we have used the `ode45` Runge-Kutta scheme to perform the numerical integration in time. We now present the results of these simulations and discuss their implications.

3 RESULTS AND DISCUSSION

For investigation into the damping characteristics of a grain boundary modeled as a dislocation array, we use the following parameters. This is what we will refer to as a standard oscillator:$L = 1\mu$m, $h = w = L/10$, $B = 10^{-4}$ Pa-s, mode = 1. Our objective has been to examine the effect of the misorientation angle and the geometry of the interface on the total damping in the system. The misorientation angle (θ) is varied from $5° - 35°$ and the Q is computed for every such angle. Other parameters such as the geometry of the beam and boundary, material properties, etc are held fixed as in the standard oscillator. Also the inclination angle (α) is varied by rotating the grain boundary about the centroid of the beam always ensuring that the midpoint of the interface coincides with the centroid of the beam. For each of the pairs of angles (θ,α) we have plotted the Qs in fig.3.

Two observations in this plot are noteworthy. We find that the quality factor steadily drops from about 2×10^4 to about 500 as θ increases. This means that dissipation) can be subtracted from the measurement.

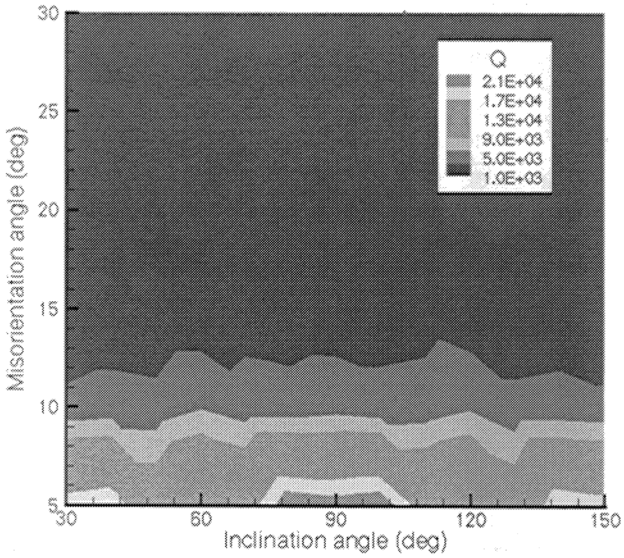

Figure 3: Variation of Q on inclination angle (α) and misorientation angle (θ) in a standard oscillator.

high angle grain boundaries are prone to dissipate more energy than their low angle counterparts. Recall from eq. (6) that the number of dislocations N is directly proportional to the angle θ. An increase in θ leads to an increase in number of oscillators i.e. it leads to an increase in the total viscous damping in the system. Since Q is inversely proportional to the total dissipation, it is expected that it will drop as N increases. Fig. 3 thus confirms this behavior. We find that the quality factor is higher for low misorientation angles (θs) than for high θs. However, an interesting feature of fig.3 is that $Q(\theta, \alpha)$ for a fixed θ fluctuates as the inclination angle α is varied from $30° - 150°$. For example, when $\theta = 5°$, we find that $1 \times 10^3 \leq Q(5, \alpha) \leq 2 \times 10^4$. This behavior is attributable to a change in the properties of the system namely its number of degrees of freedom N, stiffness K, and excitation f in eq. (12) being functions of the inclination angle α.

Upon comparing the quality factors due to the mechanism of interfacial motion with those associated with other mechanisms [2], we find that they lie in the same range, $10^3 - 10^5$. More importantly, this also means that experiments have to be very carefully designed to pick out individual mechanisms which give rise to these different Qs. We propose that an experiment involving the measurement of Q of two oscillators identical in all respects except that one being adulterated with a grain boundary would be worthwhile. This would help in zeroing on the dissipation attributable to the grain boundary alone since all other factors (the background

4 CONCLUSION

In this paper, we have investigated the role of low angle tilt grain boundaries as energy dampers in resonating micro-beams. The grain boundary was modeled as an array of edge dislocations whose simulated dynamics led to the computation of the mechanical quality factor Q. We presented results showing the explicit dependence of Q on the misorientation (tilt) angle which is an important microscopic parameter characterizing the grain boundary. Our computations showed that dissipation solely due to the mechanism of interfacial motion has Q in the range of $10^3 - 10^4$ depending on the angle of inclination between the grain boundary and the longitudinal axis of the beam. We believe that this is effect is significant and a technologically relevant one, and merits further experimental attention.

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