# Stress concentrations, diffusionally–accommodated grain boundary sliding and the viscoelasticity of polycrystals

L.C. Lee<sup>†</sup>, S.J.S. Morris<sup>†</sup>, J. Wilkening<sup>‡</sup>

 $^\dagger$  Department of Mechanical Engineering, University of California, Berkeley 94720

<sup>‡</sup> Department of Mathematics, University of California, Berkeley 94720

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#### Abstract

Using analytical and numerical methods, we analyze the Raj–Ashby bicrystal model of diffusionally accommodated grain–boundary sliding for finite interface slopes. In that model, two perfectly elastic layers of finite thickness are separated by a given fixed spatially periodic interface. Dissipation occurs by two processes: time–periodic shearing of the interfacial region; and time–periodic diffusion of matter along the interface. Though two timescales govern these processes, of particular interest is the characteristic time  $t_D$ taken for matter to move by grain–boundary diffusion over distances of order the grain size. Two previously unrecognized features of the loss spectrum in the seismic frequency band  $\omega t_D \gg 1$  are established here. First, we show that if all corners on the interface are geometrically identical, the mechanical loss  $Q^{-1}$  depends on angular frequency  $\omega$  by a strict power law  $Q^{-1} = \text{const.}\omega^{\alpha}$ . For two sliding surfaces found in a regular array of hexagonal grains, the exponent  $\alpha \sim -0.3$ . Second, our analysis shows that  $\alpha$  decreases slowly as  $\omega$  is increased if corner angle varies along the interface. Ultimately  $Q^{-1}$  is controlled by the corner having the most singular stress behaviour. Though these results are obtained from the idealized bicrystal model, we argue physically that similar behaviour will be found in numerical models of polycrystals.

### 1 **1** Introduction

Motivated by the problem of seismic attenuation, the mechanical loss spectrum of fine-2 grained mantle minerals has been measured at high temperatures in forced torsional-3 oscillation experiments (e.g. Gribb & Cooper 1998; Jackson et al. 2004; Sundberg and 4 Cooper 2010). According to these experiments, within the seismic frequency range, the me-5 chanical loss  $\mathcal{L}$  (inverse of the quality factor Q) varies with angular frequency  $\omega$  according 6 to a power law:  $\mathcal{L} \propto \omega^{-\alpha}$  with  $0.2 < \alpha < 0.35$ . Gribb & Cooper (1998, §4) summarize the 7 experimental evidence supporting diffusionally-accommodated grain-boundary sliding as 8 the attenuation mechanism in these experiments. To their considerations, we can add the 9 following argument of dynamical similarity (Morris & Jackson 2009a): values of  $\mathcal{L}$  measured 10 as a function of frequency for different grain sizes and temperatures define a single curve 11 when graphed against the dimensionless frequency  $\omega \eta'/\mu$ . Here  $\mu$  is the grain rigidity, and  $\eta'$ 12 is the steady-state viscosity for Coble creep measured in independent uniaxial compression 13 tests. Because  $\eta'$  is controlled by grain-boundary diffusion, it follows that  $\mathcal{L}$  is also. (As 14 discussed by Gribb & Cooper 1998, the experiments are designed to eliminate dislocation 15 damping; grain sizes are kept sufficiently small that, within individual grains, dislocation 16 numbers are negligible for the experimental levels of shear stress.) 17

Though the experimental results can be fitted by spring-dashpot models containing a 18 sufficient number of elements, Gribb & Cooper (1998) and Cooper (2002) argue that the 19 power-law form of the spectrum can be explained more physically by accounting for the 20 spatial variation of stress within grains. To test that explanation, they use the bicrystal 21 model of grain-boundary sliding described by Raj (1975); two isotropic Hookean layers are 22 separated by a fixed prescribed non-plane interface upon which the shear stress vanishes, 23 and across which the normal velocity is discontinuous owing to (grain boundary) diffusion 24 along the interface. To determine the loss spectrum for that model, Gribb & Cooper (1998) 25 solve the initial-value problem determining the response for a step change in applied stress, 26 and then find the loss spectrum by Laplace transformation. As shown in their Fig.10, 27 the agreement between theory and experiment supports their explanation of the observed 28 power-law spectrum. 29

That agreement is called into question by recent work. Morris & Jackson (2009b) repeat 30 that calculation using the same assumption of infinitesimal grain boundary topography. The 31 new solution differs from the earlier one in two essentials: the loss spectrum is now obtained 32 directly by imposing a sinusoidally varying boundary stress; and an explicit asymptotic 33 form is obtained giving  $\mathcal{L}$  at high frequencies  $\omega \eta'/\mu \gg 1$ . According to the new solution, 34  $\mathcal{L}$  decreases much more slowly than Gribb & Cooper predicted; it does not even follow a 35 power law, but instead decays inversely with the logarithm of frequency. Thus, although 36 experimental evidence points to grain-boundary sliding as the explanation for the high-37 temperature attenuation background, detailed analysis of the simplest (bicrystal) model 38 predicts a spectrum that is qualitatively different from that observed. 39

Despite that result, we argue here that useful lessons can still be drawn from the bicrys-40 tal model, provided the effect of finite interface slopes is included. Using analytical and 41 numerical methods, we show that for the sawtooth or truncated sawtooth interfaces (the 42 mode 1 and mode 2 sliding surfaces of Raj & Ashby 1971), the bicrystal model does in-43 deed predict a power-law spectrum when the slope is finite; for  $\omega \eta'/\mu \gg 1$ , the mechanical 44 loss  $\mathcal{L} \propto (\omega \eta'/\mu)^{-\alpha}$  at high frequencies. Though the exponent  $\alpha$  is uniquely determined 45 by the angle subtended by the corner on these piecewise linear interfaces, the constant 46 of proportionality in the loss relation depends on the orientation of the interface. In the 47

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Though we establish this result for the bicrystal model, we expect a similar result should 54 apply in a three–dimensional sample. This result is, of course, a refinement of the Gribb 55 & Cooper explanation. It provides a definite picture of where dissipation is occurring; and 56 it implies that is fruitless to seek a simple theory making quantitative predictions of  $\mathcal{L}$  for 57 a three-dimensional sample. For, although the dissipation is localized, its magnitude and 58 scaling with frequency depends on the geometry of grains and corners. Cross-sections of 59 experimental samples (e.g. Barnhoorn et al. 2007, fig.1e) do not resemble that of a regular 60 hexagonal array, and the 3-dimensional geometry is likely to be even more complex. In 61 addition to providing this (negative) guide to model building, our analysis also provides 62 quantitative results suitable for testing numerical studies. 63

Following the statement  $(\S^2)$  of the boundary-value problem (b.v.p.) and outline  $(\S^3)$ 64 of our numerical method, in §4, we use scaling to show that for a sawtooth interface, 65  $\mathcal{L} \propto (\omega \eta'/\mu)^{-\alpha}$  for  $\omega \eta'/\mu \gg 1$ . As Eq.(19) we give the formula relating the power-law 66 exponent  $\alpha$  to the angle subtended by the corner on the sawtooth interface. In §5, we 67 show that our numerical results agree quantitatively with that power law. Because cross-68 sections of experimental samples show a range of corner angles, some corresponding to 69 triple junctions, while others appear to correspond to kinks in the grain boundary, we 70 then consider an interface having two different corner angles. According to our numerical 71 solutions, the slope of the loss spectrum then decreases gradually with increasing frequency; 72 at high frequency, the behaviour of the mechanical loss appears to be controlled by the 73 corner having the strongest singular stress behaviour. Consequently, one should not expect 74 a single power law to fit the entire range of experimental frequencies. This result might 75 account for the range of  $\alpha$ -values found in experimental studies. In §6, we summarize our 76 chief results and conclusions. 77

78 Throughout this work, dimensional variables are denoted by asterisks.

### <sup>79</sup> 2 Boundary-value problem

Fig. 1 shows the geometry of the bicrystal model. In the model, two perfectly elastic grains 80 with rigidity  $\mu$  and Poisson ratio  $\nu$  are separated by an interface  $S_I$ . The interface is periodic 81 with a wavelength  $2\pi/\xi$ , where  $\xi$  is the wavenumber. Because samples in the attenuation 82 experiments are subjected to small strains  $O(10^{-6})$  (Jackson *et al.*, 2004), we assume the 83 interface position to be time-independent, given by a function  $f^*(x^*)$ . Unit vectors in the 84 coordinate directions are denoted by  $\hat{\mathbf{x}}$  and  $\hat{\mathbf{y}}$ ; unit tangent and unit normal vectors of the 85 interface are denoted by  $\hat{\mathbf{s}}$  and  $\hat{\mathbf{n}}$ , respectively. Along the upper and lower boundaries at 86  $y^* = \pm a/\xi$ , the imposed displacement varies sinusoidally in time with angular frequency 87  $\omega^*$  and amplitude  $U_0$ , i.e.  $\mathbf{u}^* = \hat{\mathbf{x}} U_0 e^{i\omega^* t^*}$ . The grains are assumed to be undergoing plane 88 deformation and the x and y components of the displacement vector  $\mathbf{u}^*$  are denoted by 89  $u^*(x^*, y^*)$  and  $v^*(x^*, y^*)$ , respectively. Similarly, the Cartesian components of the stress 90 and strain tensors are denoted by  $\sigma_{ij}^*(x^*, y^*)$  and  $e_{ij}^*(x^*, y^*)$ , respectively. 91



Figure 1: Definition sketch.

On the grain interface  $S_I$ , we impose the following constitutive equations:

$$\ell \sigma_{ns}^* = \eta \left[ \dot{u}_s^* \right] \,, \tag{1a}$$

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$$[\dot{u}_n^*] + \frac{v\ell D}{kT} \frac{d^2 \sigma_{nn}^*}{ds^{*2}} = 0.$$
 (1b)

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The parameters  $\ell$ ,  $\eta$ , v, D, k and T denote boundary thickness, boundary viscosity, molecu-95 lar volume, grain boundary diffusivity, Boltzmann constant and temperature, respectively. 96 Eq. (1a) states that the shear stress along  $\mathcal{S}_I$  is proportional to the discontinuity in the 97 tangential velocity across  $S_I$ . As described by Raj & Ashby (1971), the thin disordered 98 boundary phase acts as if it contains a liquid film having uniform viscosity  $\eta$  and constant 99 thickness  $\ell$ . We may note that in connection with the steady state creep viscosity  $\eta'$  which is 100 the manifestation of diffusion at the grain scale, the boundary viscosity  $\eta$  is a manifestation 101 of diffusion at the scale of grain boundaries. Eq. (1b) is obtained by combining Fick's law 102 with interfacial mass balance. The volumetric flow rate  $j^*$  (per unit z-length) along the 103 interface due to grain boundary diffusion is related to the normal stress by  $j^* = \frac{v\ell D}{kT} \frac{\mathrm{d}\sigma_{nn}^*}{\mathrm{d}s^*}$ 104 in a form analogous to Fick's law (Lifshitz, 1963 and Raj & Ashby, 1971). Using that 105 definition of the volumetric flow rate and invoking interfacial mass balance 106

$$[\dot{u}_n^*] + \frac{\mathrm{d}j^*}{\mathrm{d}s^*} = 0 \tag{2}$$

leads to the second constitutive equation given in (1b). According to (1b), mass flows along
the interface from regions under compression to regions in tension.

Following Mosher & Raj (1974) and Raj (1975), we define the sliding timescale  $t_{\eta}$  and the diffusive timescale  $t_D$  by

$$t_{\eta} = \frac{\eta}{\xi \ell \mu}, \qquad \qquad t_D = \frac{kT}{v \ell D \mu \xi^3}.$$
 (3a, b)

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<sup>112</sup> Physically,  $t_{\eta}$  and  $t_D$  are, respectively, the timescales on which the two sides of (1a) and <sup>113</sup> (1b) balance, if derivatives along the interface scale with its wavelength. We note that

if we identify  $2\pi/\xi$  with the grain dimension d, the timescale  $t_D$  is within a factor of 2 114 of the Maxwell time  $\eta'/mu$  based on the Coble creep viscosity. According to Morris & 115 Jackson (2009a, Fig.3) for experiments in the seismic frequency range  $0.1 < \omega_* \eta'/\mu < 10^8$ , 116 and in most cases  $\omega_* \eta' / \mu \gg 1$ . Consequently, though our numerical results will cover 117 the whole range of dimensionless frequencies, the limiting behaviour at large dimensionless 118 frequencies is of particular interest. At those high frequencies, matter can diffuse along 119 the grain boundary only over a distance short compared with the grain size, before the 120 time-oscillatory stress reverses. Balancing terms in Eq.(1b), we find that matter diffuses 121 over a distance of order the diffusion length defined as follows: 122

$$\ell_d = \left(\frac{\mu v \ell D}{k T \omega_*}\right)^{1/3} \,. \tag{4}$$

From the identity  $\ell_d \xi = 1/(\omega_* t_D)^{1/3}$ , it follows that for  $\omega_* t_D \gg 1$ ,  $\ell_d \ll d$ , as claimed. Dimensionless variables (without asterisks) are defined as follows:

$$(x^*, y^*) = (x, y)/\xi,$$
 (5a)

$$\mathbf{u}^* = U_0 \mathbf{u} \,, \tag{5b}$$

$$f^* = \varepsilon f / \xi \,, \tag{5c}$$

$$\sigma_{ij}^* = \mu \xi U_0 \sigma_{ij} , \qquad (5d)$$

$$t^* = t_D t , \qquad (5e)$$

$$e_{ij}^* = \xi U_0 e_{ij} \,. \tag{5f}$$

<sup>130</sup> In Eq. (5c),  $\varepsilon$  is the characteristic slope of the interface.

<sup>131</sup> The dimensionless b.v.p. is as follows:

in grain 1 and in grain 2,

$$\nabla(\nabla \cdot \mathbf{u}) + (1 - 2\nu)\nabla^2 \mathbf{u} = 0; \qquad (6a)$$

134 on  $y = \pm a$ ,

$$u = \pm e^{\mathbf{i}\omega t} \,, \tag{6b}$$

$$v = 0; (6c)$$

136 on  $y = \varepsilon f(x)$ ,

$$\mathcal{M}\left[\dot{u}_{s}\right] = \sigma_{ns}\,,\tag{6d}$$

$$[\dot{u}_n] + \frac{\mathrm{d}^2 \sigma_{nn}}{\mathrm{d}s^2} = 0; \qquad (6e)$$

$$[\sigma_{ns}] = 0 = [\sigma_{nn}] \tag{6f, g}$$

139 on 
$$x = 2\pi$$
 and  $x = 0$ ,  
 $u(0, y) = u(2\pi, y)$ , (6h)

 $v(0,y) = v(2\pi, y)$ . (6i)

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 $_{142}$  In (6d), we define the viscosity parameter

$$\mathcal{M} = t_{\eta}/t_D \,. \tag{7}$$

When  $\mathcal{M} \to 0$  (fixed frequency), the interface becomes effectively inviscid i.e.  $\sigma_{ns} = 0$ . 143 Problem (6) is linear and time-separable because the interface is fixed. Consequently, the solution of (6) for a time-periodic boundary displacement is also time-periodic with 145 the same angular frequency  $\omega$ . In the equation of motion (6a), we take the acceleration 146 as negligibly small; that approximation is appropriate because the elastic wavelength for 147 the experimental frequencies is large compared to the sample size. Because the constitutive 148 equations (6d) and (6e) contain time-derivatives, displacements within the sample lag the 149 displacements imposed at the boundary. Consequently, the stress at the boundary lags the 150 displacement there. The resulting phase lag between the imposed boundary displacement 151 and the resultant boundary stress is the expression of dissipation occurring at the interface. 152 By solving (6), we are able to obtain the x-averaged shear stress  $\tau$  applied at  $y = \pm a$ . 153  $\tau$  is defined as 154

$$\tau(t) = \frac{1}{2\pi} \int_0^{2\pi} \sigma_{xy}(x, a, t) \,\mathrm{d}x \,. \tag{8}$$

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<sup>156</sup> The sample shear modulus G is then defined by the equation:

$$G = \tau(t)/\gamma(t) , \qquad (9)$$

where  $\gamma(t) = e^{i\omega t}/a$  is the sample shear strain. Because  $\tau$  and  $\gamma$  are both proportional to <sup>158</sup>  $e^{i\omega t}$  in (9), the modulus G is independent of t.

The mechanical loss  $\mathcal{L}$  is defined, as usual, by the equation

$$\mathcal{L} = \tan \arg G \,. \tag{10}$$

If the material can be modelled as a network of springs and dampers, the quantity defined in (10) is equal to the ratio of the loss per cycle to  $4\pi$  times the mean strain energy stored within the grains (O'Connell & Budiansky, 1978; Bland, 1960).



(a) Type S interface

(b) Type TS interface

Figure 2: Geometry of interface  $S_I$ 

<sup>163</sup> We initially consider the two types of interface illustrated in Fig. 2. These interfaces

<sup>164</sup> can be represented using piecewise linear functions defined by

$$f = \begin{cases} x/\pi\alpha & \text{if } 0 < x < \pi\alpha; \\ 1 & \text{if } \pi\alpha < x < \pi(1-\alpha); \\ (\pi-x)/\pi\alpha & \text{if } \pi(1-\alpha) < x < \pi, \end{cases}$$
(11)

where the specific values  $\alpha = 1/2$  and  $\alpha = 1/4$  correspond to a type S and a type TS interface, respectively. To relate the characteristic slope  $\varepsilon$  to the interface slope angle  $\varphi$ , we use (13a) and (13b) for the type S and the type TS interface, respectively.

$$\tan \varphi = \frac{2\varepsilon}{\pi}, \qquad \qquad \tan \varphi = \frac{4\varepsilon}{\pi}.$$
(13a,b)

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These interfaces are found in a regular array of hexagonal grains. In that array, the slope angles for type S and type TS interfaces have values  $\varphi = 30^{\circ}$  and  $\varphi = 60^{\circ}$ , respectively.

### <sup>171</sup> 3 Numerical method

Solving b.v.p (6) using conventional finite element method directly is challenging because boundary condition (6e) requires approximation of the second derivative of normal stress  $d^2\sigma_{nn}/ds^2$ . As a result of the stress concentration described in §4.3, numerical approximation of the term  $d^2\sigma_{nn}/ds^2$  will incur a large numerical error and requires an excessively fine mesh near the corners.

To avoid computing the second derivative of the normal stress, we use the following 177 method, based on that of Sethian & Wilkening (2003). Using the principle of superposition, 178 we decompose problem (6) into two separate b.v.p.s. By doing so, we can recast the original 179 2-dimensional b.v.p into a 1-dimensional partial differential equation (p.d.e) defined along 180 the interface  $\mathcal{S}_I$ . That p.d.e is defined by a composite operator embedded with a spatial 181 differential operator originating from (6e). B.v.p (6) is solved if the eigenvalues and the 182 eigenfunctions of the composite operator are found. To avoid calculating stress derivatives, 183 the eigenvalues and the eigenfunctions are found indirectly using a constructed 'pseudo-184 inverse' of the composite operator. The solution procedure is described in the Appendix 185 and the details are given in Sethian & Wilkening (2003) and in Lee (2010). 186

#### <sup>187</sup> 4 Asymptotes to the loss spectrum

<sup>188</sup> To derive the form for these asymptotes, we need the mechanical energy balance. According <sup>189</sup> to Morris & Jackson (2009b) and Lee & Morris (2010), for the bicrystal system shown in <sup>190</sup> Fig. 1, the external power supplied at the sample boundaries is either dissipated at the <sup>191</sup> grain interface  $S_I$  or stored as strain energy within the perfectly elastic grains, i.e.

$$4\pi\tau \frac{\mathrm{d}U}{\mathrm{d}t} = \dot{\Upsilon} + \frac{\mathrm{d}W}{\mathrm{d}t}; \qquad (13a)$$

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$$W = \int_{\mathcal{V}} \left\{ \frac{\nu}{1 - 2\nu} e_{kk}^2 + e_{ij}^2 \right\} \mathrm{d}\mathcal{V},\tag{13b}$$

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$$\dot{\Upsilon} = \int_{\mathcal{S}_I} \left\{ \frac{1}{\mathcal{M}} \sigma_{ns}^2 + \left( \frac{\mathrm{d}\sigma_{nn}}{\mathrm{d}s} \right)^2 \right\} \mathrm{d}s \tag{13c}$$

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define the strain energy function W(t) and the dissipation rate  $\dot{\Upsilon}(t)$ . Here,  $\mathcal{V}$  is the combined volume of grain 1 and 2, and  $\tau$  is the *x*-averaged shear stress defined in (8). As noted in §2, we are taking the grain interface to be time-independent throughout this work.

Before considering the power-law behaviour that is the main topic of this work, we note 198 two results from previous papers. First, according to Morris & Jackson (2009b, Eq.53), for 199  $\omega \ll 1, \mathcal{L} \propto \omega^{-1}$ . This result can interpreted as stating that for  $\omega \to 0$ , the quality factor 200  $Q = \mathcal{L}^{-1}$  is proportional to  $\omega$ , as one might expect from Taylor's theorem. Secondly, owing 201 to the slip viscosity in Eq.(1a),  $\mathcal{L}$  may have a local maximum describing the loss allowed 202 by elastically-accommodated grain-boundary sliding. As discussed by Morris & Jackson 203 (2009b), for  $\mathcal{M} \ll 1$ , that local maximum occurs at a large frequency,  $\omega = O(\mathcal{M}^{-1})$ . At 204 these very large frequencies, the background loss caused by diffusion becomes negligibly 205 small, so that the structure of the resulting loss maximum is as described by Lee & Morris 206 (2010).207

The power-law spectrum discussed in §1 occurs for  $\mathcal{M} \to 0$  ( $\omega$  fixed and large). Let 208 us consider how the b.v.p. (6) now simplifies. According to Eq.(6d), the shear stress now 209 vanishes on the interface:  $\sigma_{ns} = 0$ . The mass balance expressed by Eq.(6e) also simplifies. 210 According to Eq.(4), the terms on the left side of Eq.(6e) balance on the dimensionless 211 length scale given by  $\ell_d \xi = \omega^{-1/3}$ . Because this scale vanishes with increasing  $\omega$ , at any 212 fixed distance from a corner, diffusion along the interface becomes negligibly small, and 213 Eq.(6e) simplifies to  $[u_n] = 0$ . According to this discussion, for  $\omega$  fixed and large, and at 214 distance r from the corner that is fixed (possibly small), the interfacial conditions simplify 215 to  $[u_n] = 0 = \sigma_{ns}$ . These are the boundary conditions imposed by Picu & Gupta (1996) in 216 their local analysis of the stress state near a triple junction. According to their analysis, 217 the interfacial normal stress  $\sigma_{nn}$  is given by 218

$$\sigma_{nn} \propto r^{-\lambda} \,. \tag{14}$$

The stress exponent  $\lambda$  is independent of material properties, and depends only on corner angle; it satisfies the condition  $1 > \lambda > 0$ . The first inequality ensures that the strain energy is finite, and the second inequality follows because stress is singular at a corner.



Figure 3: Definition sketch for corner singularity.

We use this stress field to estimate the dissipation and strain energy. Because diffusion acts to smooth the stress singularity at dimensionless distance  $r_{\ell} \sim \omega^{-1/3}$ , we estimate the corresponding integrals by excluding a small neighbourhood of radius  $r_{\ell}$  centred on the corner. This cut-off length  $r_{\ell}$  determines the form of the loss spectrum. Using (14) to evaluate Eqs (14b), (14c), we find that

$$W \sim \int_{r_{\ell}}^{1} \sigma_{nn}^2 r \, \mathrm{d}r \sim 1 - r_{\ell}^{2(1-\lambda)} \,,$$
 (15a)

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$$\Upsilon \sim \frac{1}{\omega} \int_{r_{\ell}}^{1} \left( \frac{\mathrm{d}\sigma_{nn}}{\mathrm{d}r} \right)^2 \,\mathrm{d}r \, \sim \frac{1}{\omega} r_{\ell}^{-(1+2\lambda)} \,. \tag{15b}$$

We note that in Eq. (15a), the integration is carried out over an annular region, so that the area element scales as  $r \, dr$ . Because  $\lambda < 1$ , we see that W approaches a limit as  $r_{\ell} \to 0$ ; the strain energy W is not concentrated near the corner. By contrast, the dissipation is focused into the corner region, and its magnitude is controlled by the cut-off scale. Substituting for  $r_{\ell}$ , we find that  $\Upsilon \sim \omega^{2(\lambda-1)/3}$ . Using the energetic interpretation of mechanical loss  $\mathcal{L}$ given below (10), we obtain

$$\mathcal{L} \sim \omega^{-\alpha} \tag{16a}$$

236 where

$$\alpha = \frac{2}{3} \left( 1 - \lambda \right) \,. \tag{16b}$$

Because  $\lambda$  depends on corner angle, so too does  $\alpha$ . Eq. (16) holds for both interfaces 238 shown in Fig.2, with one exception. A type S interface with slope angle  $\varphi = \pm 45^{\circ}$  coincides 239 with the principal axes of stress for simple shear (Lee & Morris 2010). As a result, at 240 the high frequencies at which the simplified boundary conditions apply, grains can deform 241 under simple shear. The entire stress field is then independent of r, and the stress exponent 242  $\lambda = 0$ . Substituting that value into (16), we find that  $\mathcal{L} \sim \omega^{-2/3}$ . We note that although, 243 in this special case, the Picu & Gupta analysis still predicts a non-zero value for the 244 stress exponent, the boundary conditions ensure that the amplitude of the corresponding 245 eigenfunction is zero. We return to this point in the next section. 246

Fig. 4 summarizes the results given above. If the frequencies defining each region of the spectrum are widely separated (i.e.  $1 \ll \omega \ll \mathcal{M}^{-1}$ ), the mechanical loss  $\mathcal{L}$  should scale accordingly as defined in the figure.



Figure 4: Schematic of the mechanical loss spectrum; for the asymptote for  $\omega \mathcal{M} \gg 1$ , see Lee & Morris (2010).

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In addition to predicting the high-frequency asymptote to the loss spectrum for an 250 inviscid interface, the scaling argument above also implies that the stress near a corner 251 should be self-similar. For within the corner region, both terms in the interfacial mass 252 balance (6e) must be of comparable magnitude; moreover, the stress within that inner 253 region must match to the outer stress field given by Picu & Gupta. Using Eq.(14), and the 254 cut-off scale  $\ell_d$ , we see that values of the interfacial normal stress  $\sigma_{nn}$  computed without 255 approximation as a function of distance r from the corner should define a single curve 256 when graphed using the similarity variables  $\sigma_{nn}\omega^{-\lambda/3}$  and  $r\omega^{1/3}$ . This prediction of self-257 similarity allows another test of the arguments underlying the power-law spectrum; it is 258 verified in the next section. 259

| $\varphi$    | $\alpha$ | $\lambda$ | $\lambda_{PG}$ |
|--------------|----------|-----------|----------------|
| $18^{\circ}$ | -0.17    | 0.75      | 0.79           |
| $30^{\circ}$ | -0.3     | 0.55      | 0.60           |
| $45^{\circ}$ | -0.66    | —         | —              |
| $58^{\circ}$ | -0.49    | 0.26      | 0.26           |

Table 1: Comparing the stress exponent  $\lambda$  derived from the loss spectrum with the value  $\lambda_{PG}$  of Picu & Gupta (1996, Fig.5). See text for explanation.

#### <sup>260</sup> 5 Comparison with numerical solutions

We show results for  $0.1 < \omega < 10^8$ , corresponding roughly to the range of dimensionless frequencies encountered in the experiments (e.g. Morris & Jackson 2009a, Fig.3). Results are given for Poisson ratio  $\nu = 0.3$ , comparable to that measured in olivine (Christensen, 1996); our conclusions are insensitive to this choice.

Fig. 5 shows that, as stated in  $\S1$ , the mechanical loss spectrum is sensitive to the 265 slope angle. For this figure, we have set  $\mathcal{M} = 0$ , so that the interface is inviscid. First, 266 consider, the top curve (slope angle  $\varphi = 0.36^{\circ}$ ); for  $\omega > 0.2$ , that curve agrees closely 267 with the small-slope, high-frequency asymptote given by Morris & Jackson (2009b, Eq.39). 268 Because that portion of the curve has been obtained by two independent methods, without 269 use of adjustable constants, the agreement provides a test of our numerical method; it also 270 confirms the analysis of Morris & Jackson. The remaining curves ( $\varphi \geq 18^{\circ}$ ) show that, 271 for the range of  $\omega$  shown,  $\mathcal{L}$  decreases strongly with increasing slope angle; specifically, 272 increasing  $\varphi$  from 0.36° to 30° reduces  $\mathcal{L}$  by about a factor of 10. 273

To verify the power-law scaling given by (16), we note that for the larger values of 274  $\varphi \geq 18^{\circ}$  shown in the figure,  $\mathcal{L}$  varies as  $\omega^{-}\alpha$  for  $\omega \gg 1$ . In Table 1, we give the values 275 of  $\alpha$  obtained by fitting Eq.(19a) to the computed spectrum. The  $\lambda$  shown in column 3 276 of that table are calculated using (16). Because the normal stress distribution for a type 277 S interface is exactly an odd function with respect to the corner, these stress exponents  $\lambda$ 278 can be compared to the eigenvalues  $\lambda_{PG}$  associated with an anti-symmetric eigenfunction 279 given by Picu & Gupta (1996, Fig. 5). Comparing columns 3 and 4 of the table, we see 280 that the computed stress exponents  $\lambda$  agree closely with those obtained from the Picu & 281 Gupta analysis, except when  $\varphi = 45^{\circ}$ . As explained below (16), for that special case,  $\lambda = 0$ 282 and  $\mathcal{L} \sim \omega^{-2/3}$ . That prediction is verified in column 2 of the table. (We do not display 283 the corresponding values of  $\lambda$  and  $\lambda_{PG}$  because, as discussed in §4 above, in this case, they 284 correspond to different eigenfunctions.) The next figure is used to verify the property of 285 self-similarity discussed at the end of  $\S4$ . 286

Fig. 6 shows the interfacial normal stress  $\sigma_{nn}$  near a corner as a function of distance 287 r along the interface, with  $\omega$  as a parameter. The figure verifies the self-similarity of the 288 stress field. We also note that for the type S interface,  $\sigma_{nn}$  is an odd function of distance 289 along the interface; for this reason,  $\lambda_{PG}$  values cited in table 1 were obtained using the curve 290 given in Fig.5 of Picu & Gupta for an antisymmetric stress field. (We note that the curve 291 labels are interchanged in their figure; the solid line should correspond to the antisymmetric 292 eigenfunction.) The next two figures show the relation between the loss-maximum occurring 293 when  $\mathcal{M} \neq 0$ , and the background spectrum discussed above. 294

Fig. 7 shows the rigidity G computed as a function of angular frequency  $\omega$  with  $\mathcal{M}$  as a parameter for a type S interface with  $\varphi = 30^{\circ}$ .

Fig. 7a shows  $\mathcal{L}$  as a function of  $\omega$  for a viscous interface. In the curve for  $\mathcal{M} = 10^{-8}$ , all



Figure 5: Mechanical loss  $\mathcal{L}$  as a function of angular frequency  $\omega$  when the interface is inviscid  $\mathcal{M} = 0$ . Type S interface. N = 500. .... asymptotes Eq. (16) with  $\lambda$  given in Table 1. ----- Morris & Jackson (2009b, Eq. 39b). For other parameters, see caption to Fig. 7.

the features summarized in Fig.4 are present: for  $\omega \ll 1$ , the mechanical loss  $\mathcal{L}$  varies as  $\omega^{-1}$ ; 298 for  $1 \ll \omega \ll 10^5$ , follows the power-law asymptote discussed above; the local maximum 299 due to elastically-accommodated grain-boundary sliding is found at  $\omega \sim 10^{-8}$ ; thereafter, 300  $\mathcal{L}$  varies as  $\omega^{-1}$ , as shown in Fig.4. At the local maximum  $\mathcal{L} \simeq 0.05$ , approximately 301 equal to the value found in Lee & Morris (2010, Fig.9) for the same values of the control 302 parameters. Though we do not show loss spectra for other values of  $\mathcal{M}$  we note that once 303 the maximum is clearly visible, its height is independent of  $\mathcal{M}$ ; that is because the loss due 304 to diffusionally-accommodated sliding is then small at the peak frequency. 305

The curve for  $\mathcal{M} = 10^{-3}$  is included to show that, when the sliding timescale and the diffusion timescale are not widely separated, the loss decreases rapidly with increasing frequency, except for a short plateau covering a couple of decades in frequency.

Fig. 7b shows the sample rigidity |G|. From the curve for  $\mathcal{M} = 10^{-8}$ , we see that 309 the response consists of two regions of constant |G| separated by transition regions. The 310 first plateau covers the range  $10^2 < \omega < 10^7$ . Within this frequency range,  $\mathcal{L}$  follows the 311 power-law asymptote, the shear stress vanishes over most of the interface; because only 312 normal stresses act on the interface, |G| is less than the unit rigidity of the grains. The 313 second plateau occurs for  $\omega > 10^8$ . At these high frequencies, the grains behave as if they 314 are welded at the interface i.e.  $[u_n] = 0$  and  $[u_s] = 0$ , and  $|G| \to 1$ . Similar behaviour is 315 predicted by the small–slope analysis (Morris & Jackson 2009b). 316

Fig. 8 shows the corresponding results for the type TS interface. They are included to show that the slowly-varying region in the mechanical loss spectrum depends on corner orientation, as well as on the angle subtended by the corner. For this type TS interface with  $\varphi = 60^{\circ}$ , the subtended angle is identical with that of the type S interface discussed



(c) Type S interface ( $\varphi = 45^{\circ}$ )

Figure 6: Normal stress  $\sigma_{nn}$  distribution near corner. Inset shows geometry. —  $\omega = 10^5$ . ----- $\omega = 10^4$ . …  $\omega = 10^3$ . (a) Type *S* interface.  $\varphi = 30^\circ$ .  $\lambda = 0.55$ . (b) Type *TS* interface.  $\varphi = 60^\circ$ .  $\lambda = 0.45$ . (c) Type *S* interface.  $\varphi = 45^\circ$ .  $\lambda = 0$ . Refer to Fig. 7 for other parameters.



Figure 7: Rigidity as a function of  $\omega$  with  $\mathcal{M}$  as a parameter. Type S interface, a = 5,  $\varphi = 30^{\circ}$ ,  $\nu = 0.3$ . (a)  $\mathcal{L} = \tan \arg G$ ; (b) |G|. Curve labels give values of  $\mathcal{M}$ . ----- asymptote  $\mathcal{L} \sim \omega^{-1}$ . .... asymptote Eq. (16). ----- asymptote  $\mathcal{L} \sim \omega^{-1}$ . Constant of proportionality is fitted for Eqs (15), (19).



Figure 8: Rigidity as a function of  $\omega$  with  $\mathcal{M}$  as a parameter. Type TS interface,  $\varphi = 60^{\circ}$ . (a)  $\mathcal{L} = \tan \arg G$ ; (b) |G|. See caption to Fig.5 for curve types.

in the previous figure. The orientation is different, however. The present figure shows that in the power-law régime,  $\mathcal{L}$  decreases more rapidly in the present case. This more rapid decay reflects the parity of the most singular allowable stress eigenfunction. According to Fig. 6(a), for the type S interface,  $\sigma_{nn}$  is an *odd* function of distance along the interface, whereas for a type TS interface,  $\sigma_{nn}$  is nearly an *even* function. Using Picu & Gupta (1996, Fig. 5), we find that for a symmetric stress eigenfunction  $\sigma_{nn}$ , the stress exponent  $\lambda = 0.45$ . The same value is obtained by fitting the values of  $\mathcal{L}$  shown in Fig. 8 to (16). We conclude that although, at high frequencies, dissipation is concentrated near grain corners, we can not predict the loss spectrum without accounting for the orientation of grain boundaries.

In cross-sections of experimental samples, corner angles of differing sizes. According to the results above, each such corner will contribute a characteristic value of  $\alpha$ . The next figure shows how two corners having different angles affect the loss spectrum.

In cross–sections of experimental samples, corner angles of differing sizes occur. It is 333 interesting to see how two corners subtending different angles affect the loss spectrum. 334 Because the strain energy W is insensitive to local stress behaviour, the mechanical loss  $\mathcal{L}$ 335 can be found by summing the contribution of the dissipation  $\Upsilon$  from each region surrounding 336 a corner. Consequently, the mechanical loss  $\mathcal{L}$  behaviour in the slowly-varying region is a 337 summation of the power-law scaling associated with each corner. The constants of each 338 scaling are determined by the respective constants of proportionality found in the Picu 339 & Gupta local stress description. Our scaling analysis suggests that the mechanical loss 340 behaviour in polycrystals at sufficiently high frequencies i.e.  $\omega \to \infty$  will be controlled by 341 the corner having the largest stress exponent  $\lambda$ . 342

To test this prediction, we consider an interface illustrated in the inset of Fig. 9 by the solid line. Along the interface, there are two different corners  $C_1$  and  $C_2$  having angles  $\phi_1 = 175^\circ$  and  $\phi_2 = 107^\circ$ , respectively. For these two corners  $C_1$  and  $C_2$ , the local analysis by Picu & Gupta (1996) predicts the strongest stress exponents  $\lambda$  to be 1 and 0.5, respectively. The behaviour of the mechanical loss  $\mathcal{L}$  at sufficiently high frequencies is therefore expected to be controlled by  $C_1$ .

Fig. 9 shows the mechanical loss spectrum obtained for the interface shown in the 349 inset. There are two main features in the figure. First, the behaviour of the mechanical 350 loss is consistent with the above prediction and appears to approach the logarithmic scaling 351 i.e.  $1/\ln \omega$  corresponding to a stress exponent  $\lambda = 1$  at  $C_1$ . The graph is truncated at 352  $\omega = 5 \times 10^8$  due to a lack of numerical resolution at higher frequencies. Second, the slope 353 decreases gradually with frequency in the slowly-varying region due to the diminishing 354 effect on the loss spectrum from the other corner  $C_2$ . To show that the effect of  $C_2$  indeed 355 diminishes with increasing frequency  $\omega$ , we also graph the scaling  $\mathcal{L} \sim \omega^{-0.33}$  produced by 356  $C_2$ . 357

This result is also consistent with the behaviour of the mechanical loss  $\mathcal{L}$  found in experiments. Because corner angles in triple junctions vary spatially within polycrystals, a gradual decrease in the slope of the mechanical loss spectrum caused by the diminishing effect from corners having smaller stress exponents  $\lambda$  is also expected to be observed in experiments. This may explain the behaviour seen in Fig.3 of Morris & Jackson (2009), in which the measured quality factor  $Q = \mathcal{L}^{-1}$  becomes decreasingly sensitive to  $\omega$  at higher frequencies.

# 365 6 Conclusion

We have made an analytical and numerical study of diffusionally-accommodated grain boundary sliding along a prescribed spatially-periodic finite-slope interface using a bicrystal



Figure 9: Mechanical loss  $\mathcal{L}$  as a function of angular frequency  $\omega$  for the geometry given in the inset.  $\phi_1 = 175^{\circ}$ ,  $\phi_2 = 107^{\circ}$ . Dotted lines:  $\mathcal{L} \sim \omega^{-0.33}$  and  $\mathcal{L} \sim 1/\ln \omega$ . Refer to text for explanation.

<sup>368</sup> model. Using scaling analysis, we have derived asymptotes to the mechanical loss spectrum <sup>369</sup> and show that our numerical results agree with these asymptotes. Our results show that the <sup>370</sup> general features predicted by the small–slope analysis in the mechanical loss spectrum are <sup>371</sup> present even for a finite slope interface. Here, we summarize key features in the spectrum <sup>372</sup> for a finite–slope interface when the timescales are widely separated i.e. when  $\mathcal{M} \ll 1$ :

(i) A local maximum is found near frequency  $\omega \sim \mathcal{M}^{-1}$ . That peak stands out from the absorption (or high-temperature) background caused by diffusion.

(ii) For periodic interfaces having sharp corners subtending identical angles, a slowly– varying region of the mechanical loss  $\mathcal{L}$  is found at frequencies  $1 \ll \omega \ll \mathcal{M}^{-1}$ . Within that region,  $\mathcal{L}$  follows a power–law relation i.e.  $\mathcal{L} \sim \omega^{\alpha}$ , where  $\alpha$  depends on the stress exponent  $\lambda$  by (16). Because of the constraints to the stress exponent  $\lambda$ , the power–law exponent is bounded by  $-2/3 \leq \alpha < 0$ . The parameter  $\alpha$  depends on orientation of the sliding surfaces, in addition to the angle subtended by the corner (compare Figs 7a,8a).

Our analysis suggests that the mild variation of the mechanical loss with frequency that 382 is often seen in experiments is likely to be caused by corner stress concentrations. For the 383 type S and the type TS interfaces found in a regular array of hexagonal grains, the power 384 law exponents  $\alpha$  are found to have values -0.3 and -0.37, respectively. These values are 385 close to those observed in the experiments. Because these values are also comparable to one 386 another, we speculate that the power law exponent controlling the mechanical loss scaling 387 in a regular array of hexagonal grains is also  $\sim 0.3$ . That result still needs to be verified 388 numerically. 389

In an array of regular hexagons, corner angle is constant along a sliding surface. That is 390 not so in polycrystals which typically have a range of grain sizes and corner angles. Based 391 on the preceding analysis, we therefore expect the slope in the loss spectrum to decrease 392 with increasing frequency as the effects from the corners having weaker stress concentration 393 diminishes. That result is consistent with the experiments and suggests that the differing 394 values of power-law exponent  $\alpha$  found experimentally may reflect the differing ranges of  $\omega t_D$ 395 accessed in those experiments. In the high frequency extreme  $\omega \to \infty$ , the mechanical loss 396 scaling is predicted to be controlled by the corner having the largest stress exponent. Our 397 result supports that prediction but due to the limitation of our computational resources, 398 we are unable to verify it. The result could be verified by using a finer mesh near corners 399 or by using singularity basis function in the finite element method. 400

We have shown that the behaviour of the mechanical loss spectrum found in the at-401 tenuation experiments can be explained using the simplest physical model of diffusionally-402 accommodated grain boundary sliding. Because our results show that the loss spectrum is 403 controlled by local stress behaviour near triple junctions, our prediction should, in princi-404 ple, persist even in polycrystals. Our results can therefore be used as a check for numerical 405 models of polycrystals. To predict a general mechanical loss scaling found in polycrys-406 tals, several complications not found in this simple bicrystal model need to be addressed. 407 These complications are, namely, (i) concurrent sliding along multiple planes, (ii) random 408 distribution of crystal orientation and corner angles at triple junctions. To address these 409 complications, one may then have to resort to homogenization techniques. 410

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# <sup>490</sup> Appendix: Solution procedure

Because interface  $S_I$  is time-independent and the b.v.p. given in (6) is linear, the principle of superposition applies. We decompose that b.v.p into two separate b.v.p.'s which we denote here as b.v.p<sup>(1)</sup> and b.v.p<sup>(2)</sup>. These two b.v.p.'s share the same geometry shown in Fig. 1. Using superscripts 1 and 2 to denote, respectively, variables associated with b.v.p<sup>(1)</sup> and b.v.p<sup>(2)</sup>, the stress field  $\sigma_{ij}$ , strain field  $e_{ij}$  and the displacement fields u, v of (6) can be obtained by superposing the solution of the two b.v.p.'s, i.e.

$$\sigma_{ij} = \sigma_{ij}^{(1)} + \sigma_{ij}^{(2)},$$
 (A-1a)

$$e_{ij} = e_{ij}^{(1)} + e_{ij}^{(2)},$$
 (A-1b)

$$(u, v) = (u^{(1)}, v^{(1)}) + (u^{(2)}, v^{(2)}).$$
 (A-1c)

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To simplify the notation, we use  $g_n$  and  $g_s$  here to denote, respectively, the normal displacement jump  $[u_n]$  and the tangential displacement jump  $[u_s]$  across the interface  $S_I$ . Interfacial stresses and displacement jumps are also denoted using  $2 \times 1$  vector of functions  $\sigma_n = [\sigma_{nn}, \sigma_{ns}]^T$  and  $g = [g_n, g_s]^T$ , respectively.

The plane elastostatic equation in Eq. (6a), the periodic boundary conditions in Eqs. (6h, i) and the requirement that the normal and tangential stresses across the grain boundary are continuous in Eqs. (6f, g) all apply in  $b.v.p^{(1)}$  and  $b.v.p^{(2)}$ . The other boundary conditions are now stated. In  $b.v.p^{(1)}$ , the boundary conditions at  $y = \pm a$  are

$$u^{(1)} = \pm e^{i\omega t}, \qquad v^{(1)} = 0, \qquad (A-2a,b)$$

and the boundary conditions along the interface  $S_I$  are

$$\sigma_{ns}^{(1)} = 0$$
,  $\sigma_{nn}^{(1)} = 0$ . (A-3a,b)

507 Conversely in b.v.p<sup>(2)</sup>, boundary conditions at  $y = \pm a$  are

$$u^{(2)} = 0,$$
  $v^{(2)} = 0,$  (A-4a,b)

<sup>508</sup> whereas boundary conditions along the interface  $S_I$  are

$$\mathcal{M}\dot{g}_{s}^{(2)} = \sigma_{ns}^{(2)}, \qquad \dot{g}_{n}^{(2)} + \frac{\mathrm{d}^{2}\sigma_{nn}^{(2)}}{\mathrm{d}s^{2}} = 0.$$
 (A-5a,b)

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<sup>486</sup> 

<sup>510</sup> By inspection of b.v.p<sup>(1)</sup>, the two grains do not interact with one another through the <sup>511</sup> interface  $S_I$ . Hence, the two grains move rigidly across one another and the displacement <sup>512</sup> field **u** of the upper grain and the lower grain are  $ie^{i\omega t}$  and  $-ie^{i\omega t}$ , respectively. These dis-<sup>513</sup> placement fields satisfy all equations given in b.v.p<sup>(1)</sup>, and the resulting normal displacement <sup>514</sup> jump and tangential displacement jump across the interface  $S_I$  are, respectively,

$$g_n^{(1)} = 2e^{i\omega t} \mathbf{\hat{x}} \cdot \mathbf{\hat{n}} , \qquad \qquad g_s^{(1)} = 2e^{i\omega t} \mathbf{\hat{x}} \cdot \mathbf{\hat{s}} . \qquad (A-6a,b)$$

515 We also note that in b.v.p<sup>(1)</sup>, the stress field  $\sigma_{ij}^{(1)} = 0$ .

To solve b.v.p<sup>(2)</sup>, we use eigenfunction expansion. In essence, we reduce a 2-dimensional problem given in b.v.p<sup>(2)</sup> to a 1-dimensional problem defined along interface  $S_I$ . We define a linear operator S that maps the given displacement jumps  $g^{(2)}$  onto the interfacial stresses  $\sigma_n^{(2)}$ . Note that S solves for  $\sigma_n^{(2)}$  when  $g^{(2)}$  is prescribed along the interface  $S_I$ . Because stresses in b.v.p<sup>(1)</sup> are zero, the interfacial stresses in b.v.p<sup>(2)</sup> are equivalent to that in the original b.v.p. i.e.  $\sigma_n^{(2)} = \sigma_n = (\sigma_{nn}, \sigma_{ns})^{\mathrm{T}}$ . The operator S is defined as follows:

$$S: g^{(2)} \longrightarrow \sigma_n^{(2)}$$
. (A-7)

 $_{522}$   $\,$  We also define the differential operator L as

$$\mathsf{L}: \sigma_n \longrightarrow \left(\frac{\mathrm{d}^2 \sigma_{nn}}{\mathrm{d}s^2}, \ -\mathcal{M}^{-1} \sigma_{ns}\right)^{\mathrm{T}}.$$
 (A-8)

In Eq. (A-8), L operates separately on functions  $\sigma_{ns}$  and  $\sigma_{nn}$ ; multiplying  $\sigma_{ns}$  with  $-\mathcal{M}^{-1}$ and taking the second derivative of  $\sigma_{nn}$  with respect to s. Using the definitions given in (A-7) and (A-8), and noting that  $\sigma_n = \sigma_n^{(2)}$ , we find, from the constitutive equations (6d) and (6e) of the original b.v.p, that  $\mathsf{LSg}^{(2)} = \dot{g}$ . Applying the principle of superposition  $\dot{g} = \dot{g}^{(1)} + \dot{g}^{(2)}$ to that equation, the 2-dimensional elasticity problem is absorbed into the operators leaving a single equation governing the time–evolution of the interfacial displacement jumps:

$$\dot{g}^{(2)} + \text{LS}\,g^{(2)} = -\dot{g}^{(1)}\,.$$
 (A-9)

<sup>529</sup> The r.h.s term in (A-9) can be calculated using (A-6).

Time evolution of the interfacial gap  $g^{(2)}$  defined in (A-9) can be obtained by eigenfunction expansion if the eigenvalues  $\gamma_k$  and the eigenfunctions  $Z_k(s)$  associated with the composite operator LS are known i.e.

$$\mathsf{LS}\,Z_k(s) = \gamma_k Z_k(s)\,. \tag{A-10}$$

Using  $N_z$  eigenfunctions, the solution to the homogeneous part of (A-9) (i.e. with  $\dot{g}^{(1)} = 0$ ) is given by a separable form

$$g_h^{(2)}(s,t) = \sum_{k=1}^{N_z} \beta_k \, e^{-\gamma_k t} Z_k(s), \qquad (A-11)$$

where the subscript h refers to the homogenous solution and  $\beta_k$  are coefficients determined by the initial condition  $g_0^{(2)}(s)$ . The coefficients  $\beta_k$  can be found by requiring them to satisfy

$$\sum_{k=1}^{N_z} \beta_k Z_k(s) = g_0^{(2)}(s) \,. \tag{A-12}$$

537 Letting  $\Phi_Z$  be a  $1 \times N_z$  vector containing these eigenfunctions,

$$\Phi_Z = [Z_1(s), Z_2(s), \dots, Z_{N_Z}(s)];$$
(A-13)

and  $\Phi_Z^*$  be the adjoint operator of  $\Phi_Z$  so that  $\Phi_Z^* g_0^{(2)}$  is a  $N_z \times 1$  vector of scalars defined as

$$\mathbf{\Phi}_{Z}^{*} g_{0}^{(2)} = \int_{\mathcal{S}_{I}} \left[ Z_{1} g_{0}^{(2)}, Z_{2} g_{0}^{(2)}, \dots, Z_{N_{Z}} g_{0}^{(2)} \right]^{\mathrm{T}} \mathrm{d}s , \qquad (\mathrm{A}\text{-}14)$$

the coefficients  $\boldsymbol{\beta} = [\beta_1, \beta_2, \dots, \beta_{N_Z}]^{\mathrm{T}}$ , upon solving (A-11) for  $\beta_k$ , can be written as

$$\boldsymbol{\beta} = (\boldsymbol{\Phi}_Z^* \boldsymbol{\Phi}_Z)^{-1} \boldsymbol{\Phi}_Z^* \, g_0^{(2)} \,. \tag{A-15}$$

<sup>541</sup> Substituting (A-15) into (A-11), the latter equation can be written compactly as

$$g_h^{(2)}(s,t) = \mathsf{E}(t)g_0^{(2)}(s),$$
 (A-16)

where E(t) is defined as the evolution operator, or propagator

$$\mathsf{E}(t) = \mathbf{\Phi}_Z \ e^{-\mathbf{\Lambda}t} \ (\mathbf{\Phi}_Z^* \mathbf{\Phi}_Z)^{-1} \mathbf{\Phi}_Z^* \tag{A-17}$$

543 and  $\Lambda$  is a diagonal matrix defined as

$$\mathbf{\Lambda} = \operatorname{diag}\left[\gamma_1, \gamma_2, \dots, \gamma_{N_Z}\right].$$
(A-18)

The solution to the inhomogeneous PDE given in (A-9) can then be obtained using Duhamel's principle

$$g^{(2)}(s,t) = \mathsf{E}(t)g_0^{(2)} - \int_0^t \mathsf{E}(t-\bar{t}) \, \dot{g}^{(1)}(s,\bar{t}) \, \mathrm{d}\bar{t} \,. \tag{A-19}$$

Hence, b.v.p<sup>(2)</sup> is solved, if the eigenvalues  $\gamma_k$  and the eigenfunctions  $Z_k$  of LS defined in (A-10) are found.

The steady-state response of  $g^{(2)}$  can be obtained by setting the first r.h.s term in (A-19) to zero (because it vanishes as  $t \to \infty$ ), and setting the lower integration limits in the second r.h.s term from 0 to  $-\infty$  i.e.

$$g_{ss}^{(2)}(s,t) = -\int_{-\infty}^{t} \mathsf{E}(t-\bar{t})\dot{g}^{(1)}(s,\bar{t})\,\mathrm{d}\bar{t}\,.$$
 (A-20)

The subscript ss is used here to denote steady-state solution. Substituting (A-17) and (A-6) into (A-20) and then evaluate the resulting integral, the steady-state response of the

<sup>553</sup> displacement jump in b.v.p<sup>(2)</sup> becomes

$$g_{ss}^{(2)}(s,t) = \hat{g}_{ss}^{(2)}(s,\omega) e^{i\omega t}, \qquad (A-21a)$$

<sup>554</sup> where its frequency–response is given as

$$\hat{g}_{ss}^{(2)}(s,\omega) = -\Phi_Z \mathbf{D} \left(\Phi_Z^* \Phi_Z\right)^{-1} \Phi_Z^* g^{(1)}(s,0),$$
(A-21b)

and **D** is a  $N_z \times N_z$  diagonal matrix with its k-th component given by

$$\mathbf{D}_{k} = \frac{\omega^{2} + \mathrm{i}\omega\gamma_{k}}{\omega^{2} + \gamma_{k}^{2}}.$$
 (A-21c)

Noting that  $\sigma_n = \sigma_n^{(2)}$ , as explained above (A-7), the steady-state response of the interfacial stresses  $\sigma_{n,ss}(s,t) = \hat{\sigma}_{n,ss}(s,\omega)e^{i\omega t}$  can be calculated using the operator S i.e.

$$\hat{\sigma}_{n,ss}(s,\omega) = \mathsf{S}\,\hat{g}_{ss}^{(2)}(s,\omega)\,. \tag{A-22}$$

Integrating the *x*-projection of  $\hat{\sigma}_{n,ss}(s,\omega)$  along the interface  $S_I$  then leads to the *x*-averaged shear stress  $\tau$  defined in (8). The mechanical loss  $\mathcal{L}$  can thereafter be calculated using  $\tau$  as described in the main text. Thus for any given interface, the mechanical loss spectrum can be obtained by computing the eigenvalues  $\gamma_k$  and the eigenfunctions  $Z_k(s)$  of the operator LS. We thus reduce problem (6) into an eigenvalue problem.

To avoid computing the second derivative of  $\sigma_{nn}$ , a pseudo-inverse of LS is used, instead, to find the eigenvalues and eigenfunctions. The pseudo-inverse A has the same eigenfunctions  $Z_k(s)$  as LS, and its eigenvalues  $\zeta_k$  are related to those of LS by

$$\zeta_k = \begin{cases} \gamma_k^{-1} & \text{if } \gamma_k \neq 0\\ 0 & \text{if } \gamma_k = 0 \end{cases}.$$
(A-23)

The pseudo-inverse A is constructed using finite element methods; details are given in Lee (2010) and Sethian & Wilkening (2003).