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Elastically accommodated grain-boundary sliding: New insights from experiment and modeling

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ABSTRACT

Substantial progress is reported towards a reconciliation of experimental observations of high-temperature viscoelastic behaviour of fine-grained materials with the micromechanical theory of grain-boundary sliding. The classic Raj–Ashby theory of grain boundary sliding has recently been revisited – confirming the presence of the following features: (i) at a characteristic period τ_e much less than the Maxwell relaxation time τ_d, a dissipation peak of amplitude $\sim 10^{-2}$ and associated shear modulus relaxation resulting from elastically accommodated sliding on grain boundaries of relatively low viscosity; (ii) at intermediate periods, a broad regime of diffusionally-assisted grain-boundary sliding within which the dissipation varies with period as $Q^{-1} \sim T_o^{\alpha}$ with $\alpha \sim 1/3$, sliding being limited by stress concentrations at grain corners, that are progressively eroded with increasing period and diffusion distance; and (iii) for periods longer than the Maxwell relaxation time τ_d, diffusionally accommodated grain-boundary sliding with $Q^{-1} \sim T_o$. For periods $T_o \gg \tau_e$, laboratory dissipation data may be adequately described as a function of a single master variable, namely the normalised period T_o/τ_d. However, it is becoming increasingly clear that the lower levels of dissipation measured at shorter periods deviate from such a master curve – consistent with the existence of the two characteristic timescales, τ_e and τ_d, for grain-boundary sliding, with distinct grain-size sensitivities. New forced-oscillation data at moderate temperatures (short normalised periods) provide tentative evidence of the dissipation peak of elastically accommodated sliding. Complementary torsional microcreep data indicate that, at seismic periods of 1–1000 s, much of the non-elastic strain is recoverable – consistent with substantial contributions from elastically accommodated and diffusionally assisted grain-boundary sliding.

1. Theory of elastically accommodated grain-boundary sliding

In the classic theory of grain-boundary sliding (Raj and Ashby, 1971), the low effective viscosity of grain-boundary regions plays a vital role, as follows. At sufficiently low temperatures and short timescales of stress application, the behaviour of a stressed bi-crystal is strictly elastic (Fig. 1a). However, with increasing temperature and/or timescale of stress application, the low effective viscosity of the boundary region allows a finite amount of slip between adjacent grains. Slip on the periodic corrugated interface between the grains results in a spatially variable normal stress acting across the boundary. This normal stress is responsible for an elastic distortion of the grains that facilitates sliding by eliminating the incompatibilities in grain shape and provides the restoring force for recovery of the non-elastic strain on removal of the applied stress, so that the resulting behaviour is anelastic (Fig. 1b). The characteristic timescale τ_e for such anelastic relaxation by elastically accommodated grain-boundary sliding is given by the expression (e.g., Kê, 1947; Nowick and Berry, 1972):

$$\tau_e = \eta_{gb} d / G_U \delta = \eta_{gb} / G_U \alpha_b \qquad (1)$$

The thin grain-boundary region, of thickness δ and length in the sliding direction comparable with the grain size d (and hence of aspect ratio $\alpha_b = \delta/d$), is characterised by atomic positional disorder and, commonly, chemical complexity relative to the adjacent crystalline grains (e.g., Drury and Fitz Gerald, 1996; Hiraga et al., 2003; Faul et al., 2004). This grain-boundary region is assumed to respond to applied stress as a Newtonian fluid, in which the shear stress is the product of strain-rate and a viscosity $\eta_{gb} \ll \eta_{ss}$, the viscosity associated with steady-state diffusional creep of the polycrystal. The two viscosities are expected to have distinctive Arrhenian temperature dependencies. In Eq. (1), G_U is the unrelaxed shear modulus. Under conditions of sinusoidally time-varying shear stress, a dissipation peak and associated partial relaxation of the shear modulus are expected for an angular frequency $\omega \sim 1/\tau_e$.

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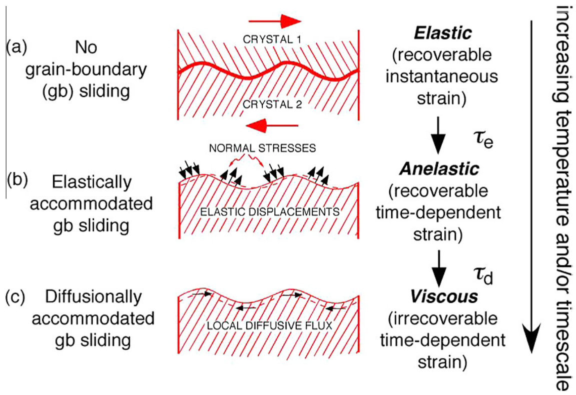

Fig. 1. The concepts that underpin the classic Raj–Ashby model of grain-boundary sliding (redrawn after Ashby, 1972). Regimes (b) and (c) are the domains of elastically accommodated and diffusionally accomodated grain-boundary sliding, respectively. Intervening between these two regimes is that of diffusionally assisted grain-boundary sliding. Within this latter regime, the distribution of boundary-normal stress is progressively modified by diffusion from that pertaining on completion of elastically accommodated sliding, involving stress concentrations at grain corners, to the parabolic distribution appropriate for steady-state creep (Raj, 1975).

At higher temperatures and/or longer timescales of stress application, the distribution of boundary-normal stress is modified by diffusional transport of matter along the grain boundary, ultimately allowing the transition from anelastic towards viscous behaviour (Fig. 1c). The time constant τ_d for the evolution of the distribution of normal stress from that prevailing on completion of elastically accommodated sliding to that associated with steady-state diffusional creep, and thus the duration of transient diffusional creep, was identified (Raj, 1975), within a dimensionless multiplicative factor, to be the Maxwell time for diffusional creep with the steady-state viscosity η_{ss}, i.e.

$$\tau_d = (1-\nu)kTd^3/(40\pi^3 G_U \delta D_{gb}\Omega) = \eta_{ss}/G_U \quad (2)$$

where ν, k, T, D_{gb}, and Ω are respectively Poisson's ratio, the Boltzmann constant, the absolute temperature, the grain-boundary diffusivity and the molecular volume of the diffusing species. Such transient creep behaviour is adequately described, at least for time intervals of finite duration, by an Andrade creep function (Gribb and Cooper, 1998; Jackson et al., 2006). For sinusoidally time-varying shear stress, such anelastic behaviour results in a weakly frequency/period dependent dissipation and associated modulus relaxation, of the type often referred to as 'high-temperature background' (e.g., Nowick and Berry, 1972).

The classical Raj–Ashby model of grain-boundary sliding has recently been revisited by Morris and Jackson (2009a). The boundary value problem describing sliding on a fixed periodic piecewise linear interface between two elastic grains, including both low effective viscosity of the grain-boundary region and grain-boundary diffusion, was solved in the limit of infinitesimal boundary slope for the complete mechanical relaxation spectrum. A dissipation peak located at $\omega \sim 1/\tau_e$, and the diffusionally accommodated sliding regime with $Q^{-1} \sim \omega^{-1}$ for $\omega < 1/\tau_d$, are separated by a diffusionally-assisted sliding regime within which Q^{-1} varies very mildly (approximately as $1/\log\omega$) with frequency (Fig. 2a). The term 'diffusionally assisted' is used to convey the idea that within this regime, diffusion occurs on progressively greater spatial scales (ultimately comparable with the grain size d) with decreasing frequency towards $1/\tau_d$. The width (in frequency or timescale of stress application) of this diffusionally assisted regime, is determined by ratio $M = \tau_e/\tau_d$, which is poorly constrained a priori, but inferred from experimental data for fine-grained polycrystals to be $\ll 1$ (Morris and Jackson, 2009a).

More recently, a combination of analytical and numerical (finite-element) methods has been used to extend the work of Morris and Jackson (2009a) to finite slopes of the same piecewise linear boundary between elastic grains (Lee and Morris, 2010;

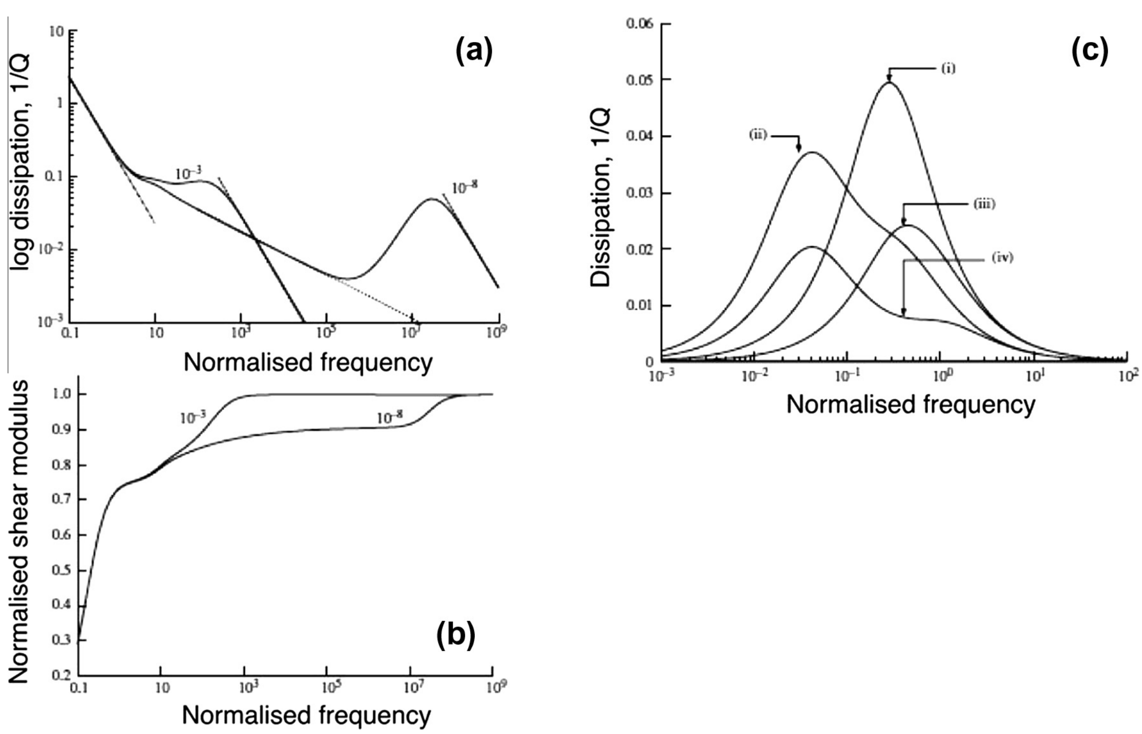

Fig. 2. (a) and (b) The mechanical relaxation spectrum of Lee et al. (2011) for the $\varphi = 30°$ saw-tooth interface, with alternative values of $M = \tau_e/\tau_d$ of 10^{-8} and 10^{-3}. (c) The effect on Q^{-1} of spatial heterogeneity in grain size and/or viscosity (Lee and Morris, 2010, Fig. 9). Curves labelled (i–iv) correspond respectively to uniform grain size and viscosity, 10-fold variation of grain-boundary viscosity, 4-fold variation of grain size, both 10-fold variation of boundary viscosity and 4-fold variation of grain size.