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Supplementary material for: Grain size assisted thermal runaway: Implications for intermediate-depth earthquake generation

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GOVERNING EQUATIONS

GRAIN SIZE EVOLUTION LAW

In this study, we use a grain size evolution law which is derived from first principles (Ricard and Bercovici, 2009) based on the assumption of a self similar and lognormal grain size distribution (Rozel et al., 2011). We will therefore shortly summarise the main properties and implications of a self similar and lognormal distribution before describing the grain size evolution law. For a more detailed derivation, we refer to Ricard and Bercovici (2009) and Rozel et al. (2011).

Self similar and lognormal grain size distribution

Inspired by various studies, Rozel et al. (2011) assume the self similarity of the grain size distribution. The number dn of grains of size \mathcal{R}' per unit volume is simply

$$dn(\mathcal{R}') = A(\mathcal{R})H\left(\frac{\mathcal{R}'}{\mathcal{R}}\right) d\mathcal{R}' \quad (\text{S.1})$$

where \mathcal{R} is the mean grain size of the distribution. This means that when normalized by its amplitude $A(\mathcal{R})$ (in m^{-4}), the distribution as a function of the normalized grain size $u = \mathcal{R}'/\mathcal{R}$ is always the same. By definition the sum of the volumes of all the grains per unit volume is 1 which implies.

$$A(\mathcal{R}) = \frac{3}{\mathcal{R}^4 \int 4\pi u^3 H(u) du} \quad (\text{S.2})$$

Observations suggest that $H(u)$ is roughly a lognormal distribution, which can be written as:

$$H(u) = \frac{1}{\sqrt{2\pi}\sigma u} \exp\left(-\frac{(\ln u)^2}{2\sigma^2}\right) \quad (\text{S.3})$$

The use of this lognormal distribution implies that

$$\int_0^\infty u^a H(u) du = \exp\left(\frac{a^2\sigma^2}{2}\right) = \lambda_a \quad (\text{S.4})$$

where a is a given real number and σ is the half-width of the lognormal distribution.

Grain boundary energy

The energy per unit volume, $e_{\mathcal{R}}$ stored in the grain boundaries of a given grain size distribution can be written as:

$$e_{\mathcal{R}} = \int_0^\infty 4\pi\gamma\mathcal{R}'^2 A(\mathcal{R})H(\mathcal{R}'/\mathcal{R}) d\mathcal{R}' \quad (\text{S.5})$$

where γ is the surface tension. Using (S.2), (S.5) can be written as:

$$e_{\mathcal{R}} = \frac{3\gamma \int_0^\infty u^2 H(u) du}{\mathcal{R} \int_0^\infty u^3 H(u) du}. \quad (\text{S.6})$$

The integrals in (S.6) can be replaced by λ_2 and λ_3 :

$$e_{\mathcal{R}} = \frac{3\lambda_2\gamma}{\lambda_3\mathcal{R}} \quad (\text{S.7})$$

Grain size evolution law

The grain size evolution law developed in Rozel et al. (2011) is written as

$$\frac{d\mathcal{R}}{dt} = \frac{\mathcal{G}}{p\mathcal{R}^{p-1}} - \frac{f_0 F_{\mathcal{R}}}{\gamma} \mathcal{R}^2 \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dis} \quad (\text{S.8})$$

where $\mathcal{G} = k_0 \exp(-Q_g/RT)$ is a growth term with a prefactor k_0 and an activation energy Q_g , $\boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}$ is the contraction of the stress and dislocation strain tensors,. $F_{\mathcal{R}} = \lambda_3/3\lambda_2$ is a constant factor which depends on the properties of the grain size distribution, with $\lambda_i = \exp(i^2\sigma^2/2)$ and σ being the half-width of the grain size distribution. f_0 (also called lambda factor or Taylor-Quinney coefficient) denotes a partitioning factor that determines how much of the work done in dislocation creep is used for grain size reduction (Austin and Evans, 2007; Rozel et al., 2011). This term varies between 0 and 1 and has to be measured in experiments and studies that indicate that it is both strain and temperature dependent (Chrysochoos and Belmahjoub, 1992; Austin and Evans, 2009; Rozel et al., 2011). We can now rearrange (S.8) to obtain an expression for the temporal change in (volume-specific) grain boundary energy $e_{\mathcal{R}}$:

$$\frac{de_{\mathcal{R}}}{dt} = \frac{d}{dt} \left(\frac{\gamma}{\mathcal{R}F_{\mathcal{R}}} \right) = f_0 \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dis} - \frac{\gamma\mathcal{G}}{pF_{\mathcal{R}}} \frac{1}{\mathcal{R}^{p+1}} \quad (\text{S.9})$$

where we assume that the surface tension is a constant, independent of temperature.

CONSERVATION OF MOMENTUM AND VISCOELASTIC RHEOLOGY

Assuming that inertial effects are negligible and that there are no body forces, conservation of momentum can be written as:

$$\nabla \cdot \boldsymbol{\tau} = 0 \quad (\text{S.10})$$

where $\boldsymbol{\tau}$ is the stress tensor. The viscoelastic rheology of the slab is modeled using a Maxwell model with shear modulus G :

$$\dot{\boldsymbol{\epsilon}} = \frac{1}{G} \dot{\boldsymbol{\tau}} + \dot{\boldsymbol{\epsilon}}_{dis} + \dot{\boldsymbol{\epsilon}}_{dif} \quad (\text{S.11})$$

where the total strain rate $\dot{\boldsymbol{\epsilon}}$ equals the sum of the elastic strain rate $\frac{1}{G} \frac{d\boldsymbol{\tau}}{dt}$ and the strain rates of dislocation creep $\dot{\boldsymbol{\epsilon}}_{dis}$ and diffusion creep $\dot{\boldsymbol{\epsilon}}_{dif}$:

$$\dot{\boldsymbol{\epsilon}}_{dis} = A_{dis} e^{-\frac{Q_{dis}}{RT}} \tau_{II}^{n-1} \boldsymbol{\tau} \quad (\text{S.12})$$

$$\dot{\boldsymbol{\epsilon}}_{dif} = A_{dif} e^{-\frac{Q_{dif}}{RT}} \mathcal{R}^{-m} \boldsymbol{\tau} \quad (\text{S.13})$$

Here τ_{II} denotes the second invariant of the stress tensor.

We can now introduce the volume-specific elastic energy $e_{el} = \boldsymbol{\tau} : \boldsymbol{\tau} / 2G$. As can be seen from (S.11), deformation of a volume element results in a change in stress and thus also in stored elastic energy. By contracting (S.11) with $\boldsymbol{\tau}$ and rearranging we obtain an expression for the temporal change in e_{el} :

$$\frac{de_{el}}{dt} = \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}} - \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dis} - \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dif} \quad (\text{S.14})$$

CONSERVATION OF ENERGY

In our model we assume that acceleration is negligible, thus the change in total energy equals the change in internal energy U . The first law of thermodynamics states that a change in internal energy in a closed system can only be achieved through either work W done by (or done to) the system or heat supplied to the system Q . In differential form, it can be written as:

$$\frac{dU}{dt} = Q - W \quad (\text{S.15})$$

where the negative sign indicates that work is done by the system. This implies that

$$\frac{dU}{dt} = \boldsymbol{\tau}:\dot{\boldsymbol{\varepsilon}} + k\nabla^2 T \quad (\text{S.16})$$

We use Fouriers law for heat flux and assume that thermal conductivity is constant. The internal energy in our system is also given by :

$$U = F + ST \quad (\text{S.17})$$

where F is the Helmholtz free energy and S the entropy. As U , F and S are volume-integrated quantities, we can rewrite (S.16) in terms of specific properties:

$$\rho\dot{f} + \rho\dot{s}T + \rho s\dot{T} = \boldsymbol{\tau}:\dot{\boldsymbol{\varepsilon}} + k\nabla^2 T \quad (\text{S.18})$$

where lowercase letters denote specific properties and $\dot{}$ denotes a time derivative. Keeping in mind that the volume of our system is constant, we can replace $s = -\partial f/\partial T$ which results in:

$$\rho\dot{f} + \rho\dot{s}T - \rho\frac{\partial f}{\partial T}\dot{T} = \boldsymbol{\tau}:\dot{\boldsymbol{\varepsilon}} + k\nabla^2 T \quad (\text{S.19})$$

In the case of viscoelastic deformation coupled with grain size evolution, the Helmholtz free energy is given by the sum of the specific elastic energy, the specific grain boundary energy and the specific thermal energy:

$$\begin{aligned} f &= \frac{e_{el}(\boldsymbol{\tau})}{\rho} + \frac{e_{\mathcal{R}}(\mathcal{R})}{\rho} + \frac{e_T(T)}{\rho} \\ &= \frac{1}{\rho} \frac{\boldsymbol{\tau}:\boldsymbol{\tau}}{2G} + \frac{1}{\rho} \frac{\gamma}{\mathcal{R}F_{\mathcal{R}}} + c_V T \end{aligned} \quad (\text{S.20})$$

With the specific Helmholtz free energy being defined, the term $\rho \dot{s}T$ in (S.19) can now be written as:

$$\begin{aligned} \rho \dot{s}T &= \rho T \frac{\partial s}{\partial \boldsymbol{\tau}} : \dot{\boldsymbol{\tau}} + \rho T \frac{\partial s}{\partial \mathcal{R}} \dot{\mathcal{R}} + \rho T \frac{\partial s}{\partial T} \dot{T} \\ &= -\frac{\partial^2 f}{\partial \boldsymbol{\tau} \partial T} : \dot{\boldsymbol{\tau}} - \frac{\partial^2 f}{\partial \mathcal{R} \partial T} \dot{\mathcal{R}} + \rho c_V \dot{T} \end{aligned} \quad (\text{S.21})$$

where we made use of $s = -\partial f / \partial T$ and $c_V = T (\partial s / \partial T)$. With our definition of the specific Helmholtz free energy, the first two terms with second derivatives on the right hand side of the above equation equal zero. Therefore using (S.20) and $\rho \dot{s}T = \rho c_V \dot{T}$, (S.19) reads as:

$$\frac{1}{G} \boldsymbol{\tau} : \dot{\boldsymbol{\tau}} - \frac{\gamma}{\mathcal{R}^2 F_{\mathcal{R}}} \dot{\mathcal{R}} + \rho c_V \dot{T} = \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}} + k \nabla^2 T \quad (\text{S.22})$$

which can be reordered to obtain:

$$\rho c_V \dot{T} = k \nabla^2 T + \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}} - \frac{1}{G} \boldsymbol{\tau} : \dot{\boldsymbol{\tau}} + \frac{\gamma}{\mathcal{R}^2 F_{\mathcal{R}}} \dot{\mathcal{R}}. \quad (\text{S.23})$$

Replacing $\boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}} = \frac{1}{G} \boldsymbol{\tau} : \dot{\boldsymbol{\tau}} + \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dis} + \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dif}$ and $\dot{\mathcal{R}}$ with (S.8) and reordering results in:

$$\rho c_V \dot{T} = k \frac{\partial^2 T}{\partial y^2} + (1 - f_0) \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dis} + \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_{dif} + \frac{\gamma \mathcal{G}}{\rho F_{\mathcal{R}} \mathcal{R}^{p+1}} \quad (\text{S.24})$$

Note that the last term is related to the grain growth term in (S.8) and \mathcal{G} is also dependent on temperature.

NUMERICAL SOLUTION

As our model consists of a viscoelastic slab sheared under simple shear, the only nonzero velocity component is in the x -direction and shear stress τ_{xy} is uniform in the slab and only dependent on time, whereas the other components of the stress tensor can be regarded as zero. By integration of (S.11) and reordering we then obtain an expression for the temporal change in shear stress:

$$\frac{d\tau}{dt} = G \left[\dot{\epsilon}_{BG} - \frac{1}{L} \int_{-L/2}^{L/2} (\dot{\epsilon}_{dis} + \dot{\epsilon}_{dif}) dy \right] \quad (\text{S.25})$$

where the background strain rate $\dot{\epsilon}_{BG} = v/L$ with v being the applied velocity difference between the top and the bottom of the slab and L the thickness of the slab. If the domain is homogeneous (S.25) reduces to:

$$\frac{d\tau}{dt} = G [\dot{\epsilon}_{BG} - (\dot{\epsilon}_{dis} + \dot{\epsilon}_{dif})] \quad (\text{S.26})$$

Likewise, the tensor contractions in (S.8) and (S.24) reduce to simple products.

0D MODEL

We define the 0D model as a model where material parameters are homogeneous and heat transfer is neglected. In this case, we have to solve a system of three coupled ordinary differential equations (S.26),(S.8) and (S.24) (in their reduced form). As the system becomes very stiff once thermal runaway occurs, we have to use a fully implicit solver to solve the system of equations. This is done using the solver *ode15i* available in the commercial software package MATLAB.

Table DR1. Rheological creep parameters used in this study (from Hirth and Kohlstedt, 2003).

Olivine flow law	A [MPa $^{-n}$ μm^m]	n	m	E_a [kJ mol $^{-1}$]
dry dislocation creep	$1.1 \cdot 10^5$	3.5	0	530
dry diffusion creep	$1.5 \cdot 10^9$	1	3	375

1D MODEL

In addition to the 0D model, we have to consider the diffusion of heat in the 1D model. This is done by discretising the domain using finite differences and computing $\partial T/\partial t$ and $\partial \mathcal{R}/\partial t$ at each node. $\partial \tau/\partial t$ is computed using (S.25), where we compute the respective strain rates at each node and then numerically integrate over the whole domain. As for the 0D model, this is done in the framework of the implicit solver *ode15i*.

MATERIAL PARAMETERS

In this study, we use different rheologies and grain growth parameters, which are listed here. For diffusion and dislocation creep, we use the rheological parameters for dry olivine given in Hirth and Kohlstedt (2003)(see tab.1). Grain growth parameters are taken from Kameyama and Yuen (1997), Hiraga et al. (2010) and Tasaka et al. (2013) (see tab.2). The remaining parameters can be found in tab.3.

INFLUENCE OF THE PARTITIONING FACTOR

In our study, we used a constant partitioning factor of $f_0 = 0.1$. To test the influence of the partitioning factor on the occurrence of thermal runaway, we also ran simulations with $f_0 = 0.5$ (which is a rather large value). In fig.S.1, we show the occurrence of thermal

Table DR2. Grain size evolution parameters used in this study.

	Parameter	Value	Unit	Name
general	γ	1	J m^{-2}	surface tension ¹
	σ	0.6		distribution half-width ²
	f_0	0.1 and 0.5		partitioning factor
pure Olivine	k_0	607	$\mu\text{m}^p \text{ s}^{-1}$	growth prefactor ³
	E_g	200	kJ/mol	activation energy ³
	p	2		growth exponent ³
Fo-En mixture	k_0	497075	$\mu\text{m}^p \text{ s}^{-1}$	growth prefactor ⁴
	E_g	300	kJ/mol	activation energy ⁵
	p	4		growth exponent ⁴

¹ Duyster and Stockhert (2001)

² Rozel et al. (2011)

³ Kameyama and Yuen (1997)

⁴ Hiraga et al. (2010)

⁵ Tasaka et al. (2013)

Table DR3. Other parameters used in this study.

Parameter	Value	Unit	Name
G	$5 \cdot 10^{10}$	Pa	elastic shear modulus
κ	10^{-6}	m^2/s	heat diffusivity
ρ	3300	kg/m^3	density
c	1050	$\text{J}/(\text{kg K})$	heat capacity

runaway for different scenarios and the corresponding stresses (compare with fig.3 in the main paper). It can be seen that f_0 does have a slight effect, but that it is rather limited, the reason being that the partitioning factor is valid for the whole domain, thus grain size reduction is also more efficient in the surrounding matrix and the relative effect of grain size reduction approximately remains the same. Note however that transient stages are affected by a different choice for f_0 , as grain size reduction is faster for larger values of f_0 (see also Herwegh et al., 2014).

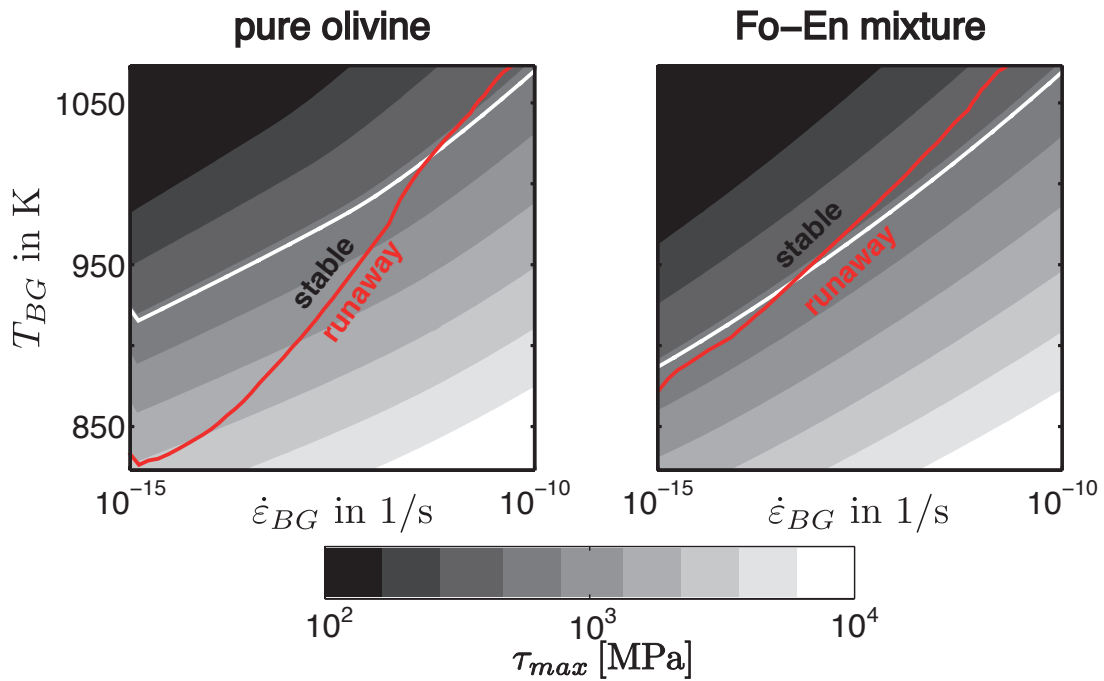


Figure DR1. Same as Fig.3, but for a partitioning factor $f_0 = 0.5$. Only slight differences can be observed compared to the results with $f_0 = 0.1$ (the crossing of the runaway regime boundary with the 600 MPa isoline occurs at slightly lower strain rates for $f_0 = 0.5$)

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