A theoretical model for the evolution of microstructure in lithospheric shear zones

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SUMMARY

The strength of the lithosphere plays a key role in the formation and evolution of tectonic plate boundaries. Localized lithospheric deformation associated with plate tectonics requires a mechanism for weakening across the entire width of the lithosphere, including the strongest cold ductile region. We explore the microphysics of weakening of lithospheric materials, and in particular the coupled evolution of mineral grain size and intragranular defects and their control on lithospheric strength. We propose a model for the interaction between grain-boundaries and dislocation density to reduce the net free energy of grains during dynamic recrystallization (DRX). The driving forces for DRX arise from heterogeneity in dislocation density and grain boundary curvature. Our model shows that grain growth driven by variation in grain boundary curvature can be impeded by variation in dislocation density; this occurs because as the grains grow, to minimize their surface energy, their dislocation density and associated internal energy may increase and offset the driving forces for grain growth. The correlation between grain size and dislocation density can, for example, arise because the dislocation accumulation in smaller grains is suppressed due to the large stress that is needed to bend and elongate a short dislocation (as dictated by the small grain size), while the larger grains can have long dislocations and reach a steady-state dislocation density dictated by the applied stress. In a lithospheric setting, slower grain growth means that it would require less mechanical work to establish weak localized shear zones through grain damage, and retard the healing of previously damaged zones. Furthermore, the competition of two different timescales—that of grain growth and the dislocation kinetics—can lead to oscillating behaviour over 1–10 yr as the grain size and dislocation density advance towards their steady states. These oscillations are likely to have an effect on the rheology of lithospheric rocks, for example, their strengthening and weakening through time, and have a potential application to geological processes such as post-seismic creep in ductile shear zones.

Key words:

1 INTRODUCTION

Deformation induced grain size reduction, or grain damage, is commonly observed in rock deformation experiments (Green & Radcliffe 1972; Karato et al. 1980; De Bresser et al. 1998), as well as natural samples, such as mylonites and ultramylonites (Kohlstedt & Weathers 1980; White et al. 1980). In fact, the measured grain size of a rock sample is commonly used as a piezometer or a paleowattmeter, that is, a quantity from which the deformation conditions (such as stress or work rate) can be inferred (Van der Wal et al. 1993; Austin & Evans 2007; Rozel et al. 2011; Mulyukova & Bercovici 2017). In lithospheric settings, the mechanical weakening of damaged material has been proposed as a mechanism for strain localization, resulting in the formation of deep lithospheric ductile shear zones (Tullis & Yund 1983; Montési & Hirth 2003; Landuyt & Bercovici 2009; Mulyukova & Bercovici 2017), or even new tectonic plate boundaries (Bercovici & Ricard 2005; Landuyt et al. 2008; Bercovici & Ricard 2012, 2013, 2014; Mulyukova & Bercovici 2018). It is worth noting that while grain damage is potentially an important plate generation mechanism, it is likely that the effects of brittle deformation, viscoplastic rheologies, lubrication by fluids and potentially other processes also play an important role, especially at shallower depths (Lenardic & Kaula 1994, 1996; Kameyama et al. 1997; Moresi & Solomatov 1998; Tackley 2000; Regenauer-Lieb et al. 2001; Bercovici & Ricard 2003; Korenaga 2007; van Heck & Tackley 2008; Foley & Becker 2009; Bercovici et al. 2015; Foley 2018).

The grain size of a material changes as a result of diffusion-driven grain growth, or, for deforming materials, in a process known as dynamic recrystallization (DRX). The microphysics of DRX largely
revolves around the dynamics of intragranular defects, namely dislocations (Urai et al. 1986; Derby & Ashby 1987; De Bresser et al. 2001). The energy associated with dislocations can give rise to a ‘thermodynamic force’ that induces grain boundary migration, which is one of the mechanisms by which dynamic recrystallization can occur. (We note that the DRX can also occur by rotation of subgrains (Guillope & Poirier 1979), but, for simplicity, we do not consider this mechanism in this paper.) That dynamic recrystallization accompanies deformation during dislocation creep is supported by experimental (Green & Radcliffe 1972) as well as theoretical (Derby & Ashby 1987) studies.

Forces that drive grain boundary migration and recrystallization can stem from the contrast in dislocation density (Guillope & Poirier 1979; Urai et al. 1986; Derby & Ashby 1987), as well as the variation in grain boundary energy (through boundary curvature, or grain size; Lifshitz & Slyozov 1961; Hillert 1965; Evans et al. 2001; Ricard & Bercovici 2009). The two forces can interact and their combined effect is likely to be reflected in the sizes of the recrystallized grains. In the following, we present a theoretical model for grain size evolution, where the driving forces for grain growth and dynamic recrystallization arise from heterogeneities in grain boundary curvature as well as dislocation density.

2 THEORETICAL MODEL OF GRAIN SIZE AND DISLOCATIONS DYNAMICS

2.1 Grain size

We consider a granular material undergoing deformation due to an applied deviatoric stress tensor ($\tau_{ij}$) and microstructural development characterized by evolving grain size ($R$) and dislocation density ($\omega$). A grains geometry is described by $R$, which for spherical grains (or even regular polyhedral grains; Ricard & Bercovici 2009) represents radius (as assumed in this paper). A single grain’s volume, surface area and grain boundary curvature are given by, respectively,

$$V = \frac{4}{3} \pi R^3$$

$$A = 4\pi R^2$$

$$K = \frac{2}{R} = \frac{dA}{dV} = \frac{2}{3} \frac{dR}{V}$$

Using the above, and assuming that the density $\rho$ is equal for all grains, mass is given by

$$\dot{m} = \dot{V} \rho = \frac{4}{3} \pi R^3 \rho$$

For the remainder of this paper, we will use the ‘ breve’ accent to denote grain-specific properties (other than for $R$), for example, each grain has a volume $\check{V}$.

A grain boundary shared between two grains of different sizes has a force acting on it, which is proportional to the pressure difference caused by its curvature, or, in other words, the difference in free energy associated with surface tension in grains of different sizes (e.g. Lifshitz & Slyozov 1961; Hillert 1965; Ricard & Bercovici 2009). This force induces grain boundary migration inward or outward from the grain. A grain grows if the averaged migration of its boundary is outward. Since the grain boundary curvature is determined by grain size (3), it follows that the size of the grain (relative to the other grains) matters for whether the grain will shrink or grow. Moreover, the rate at which the size of a grain changes is proportional to the difference between its size and that of other grains, as will be shown in detail in Section 3.

A grain that grows does so at the cost of other grains shrinking, by conservation of mass (or volume, since we assume a constant material density $\rho$), which would lead to an ever increasing difference between grain sizes, and thus increasing pressure on the grain boundary to spur on further, potentially unimpeded, grain growth. In contrast, natural rocks are clearly polycrystalline, that is, exhibit finite grain sizes rather than one single crystal. To limit grain growth in static conditions, earlier theoretical models have considered the effect of secondary phases, which can offset the pressure that drives grain boundary migration (Hillert 1965; Bercovici & Ricard 2012).

For single-phase materials, Hillert (1965) invoked topological rules for the average and minimum number of neighbours that a grain can have, which served as constraints for more realistic grain growth models.

For non-static conditions, there is another contribution to pressure acting on the grain boundary and affecting grain growth, namely the contrast in free energy associated with intragranular defects (in our case—dislocations), which accompany plastic deformation and which we describe in Section 2.2. The finite steady-state grain size in a deforming and dynamically recrystallizing material can be predicted by considering the balance in the nucleation and annihilation rates of dislocations (Derby & Ashby 1987), or by the balance between the rate of deformational work and the rate at which energy is being stored and released at newly forming or vanishing grain boundaries, respectively (Bercovici & Ricard 2005; Austin & Evans 2007; Rozel et al. 2011). We propose a new model for grain size evolution in a deforming and recrystallizing single-phase material, which explicitly considers the forces driving grain boundary migration, and as such is more readily comparable to the original models of normal grain growth discussed above. In the new model, the effect of deformation on stabilizing grain growth is treated as an additional component of pressure acting on the grain boundary, analogous to the treatment of secondary phases in the grain growth models of (Hillert 1965). Moreover, accounting for the role of deformational work on the developing microstructure, namely dislocation density, allows for a more direct comparison between our theory and experiments.

2.2 Dislocation density

The presence of dislocations induces internal stresses within the grain. Adopting the limit of linear elasticity, we assume that the stresses caused by external and internal sources can be superposed (e.g. Anderson et al. 2017, Chapter 2), and similarly for strains. Furthermore, we assume that the medium is isotropic, such that the strain energy associated with dislocations effectively acts to increase the internal pressure of the grain (and thus the grains internal energy), but does not introduce anisotropy, such that the strain rate $\dot{\epsilon}$ in response to the external deviatoric stress $\tau_{ij}$, is also isotropic. Although individual mineral grains or crystals have anisotropic properties, deformation of a grain by dislocation creep involves multiaxial movement on different slip planes [e.g. at least five independent slip systems are required for a crystal to achieve an arbitrary plastic strain (Anderson et al. 2017, Chapter 9)]. Thus, on the continuum scale, deformation of a polycrystalline material consisting of many randomly oriented grains, can still be effectively isotropic.
The anisotropic effects may still manifest on the grain scale, as dislocation motion along different slip planes can contribute a different amount to the total grain strain. Different grains can have different crystal lattice orientations. Thus, the stress tensor $\tau_{ij}$ is projected, or ‘resolved’, differently onto different grains. In particular, the slip systems activated to accommodate deformation of one grain will have a different amount of stress projected onto them than in another grain, although both grains experience the same applied stress. In addition, one can envision that in a polycrystalline domain some grains may bear more of the stress load than others, for example, due to grain size, shape or position within the domain. In total, we use the fourth rank tensor $\mathbf{T}$ to express the stress variation between the grains, such that $\tau = \mathbf{T} : \varepsilon$, and assume that the second invariants of $\varepsilon$ and $\tau$ are related as

$$\varepsilon = \mathbf{C} : \varepsilon, \quad (5)$$

where $\mathbf{C}$ is a grain-specific scalar factor, such that $0 \leq \mathbf{C} \leq 1$.

The contribution $d\epsilon_{\omega}$ to a grain’s internal energy due to a change in total length $dL$ of all dislocations contained within a grain is

$$d\epsilon_{\omega} = \gamma_{\omega} dL = \gamma_{\omega} \frac{dL}{dv}, \quad (6)$$

where we define the dislocation density:

$$\dot{\omega} = \frac{dL}{dv}, \quad (7)$$

and the energy per unit length of a dislocation:

$$\gamma_{\omega} = Gb^2, \quad (8)$$

where $G$ is the shear modulus and $b$ is the length of the Burgers vector (see Table 1). For simplicity, we assume that $\gamma_{\omega}$ is constant.

When the material deforms by dislocation creep, the strain is accommodated by the propagation of dislocations through the grain. As the material deforms, new dislocations get nucleated or elongated at a rate $\dot{\omega}^+$, move through the grain at velocity $v_{\omega}$, and get annihilated at a rate $\dot{\omega}^-$ either by merging with other dislocations or by reaching the grain boundary. The dislocation density $\dot{\omega}$ evolves in response to the competition between $\dot{\omega}^+$ and $\dot{\omega}^-$, and reaches a steady state when $\dot{\omega}^+$ and $\dot{\omega}^-$ balance each other.

The rates $\dot{\omega}^+$, $\dot{\omega}^-$, and $v_{\omega}$ depend on the specific mechanisms by which the dislocation dynamics occurs, and which in turn depend on the crystal structure of the material and the external physical conditions (e.g. stress and temperature; see Karato 2008, Chapter 9). Moreover, due to the long-ranging internal strain and stress fields associated with the dislocations, as well as their relatively large geometrical extent, the rates of processes governing dislocation dynamics depend nonlinearly on dislocation density itself (Karato 2008, Chapter 5). For example, the rate of dislocation motion $v_{\omega}$ is sensitive to the external stress, as well as the internal stress due to the presence of other dislocations (thus $\dot{\omega}$) and grain boundaries (thus $R$). It is the non-trivial dependence of $v_{\omega}$ on stress and $\dot{\omega}$ (which is itself stress-dependent), that makes for a non-linear rheology when material deforms by dislocation creep (Karato 2008, Chapter 9). Furthermore, to nucleate a dislocation or to increase the length of an existing one requires the presence of lattice imperfections such as grain or sub-grain boundaries or other dislocations. Such lattice defects can serve as nucleation sites for new dislocations, or make the motion of the existing dislocations heterogeneous, which leads to their elongation. Thus, $\dot{\omega}^+$ depends on both $\dot{\omega}$ and $v_{\omega}$. When dislocations annihilate by merging with each other, $\dot{\omega}^-$ is determined by the time it takes for a mobile dislocation to collide with another one, which depends on $\dot{\omega}$ and $v_{\omega}$. When annihilation happens at the grain boundary, then the grain size $R$ also plays a role in determining $\dot{\omega}^-$. The relationship between grain size and dislocation density can be inferred from some theoretical considerations. Consider, for example, the process of dislocation multiplication through Frank-Read sources (Anderson et al. 2017, Chapter 20). The minimum stress $\tau_{FR}$ required to bend and elongate a dislocation that is pinned at its ends (the pins can e.g. be sites where the dislocation leaves the glide plane, or some other lattice heterogeneities that inhibit dislocation motion) scales inversely with the dislocation length $L$ (Anderson et al. 2017, Chapter 20):

$$\tau_{FR} = C_{FR} \frac{Gb}{L}, \quad (9)$$

where $C_{FR}$ is a constant that depends on the type of dislocation (e.g. edge or screw), typically of order unity. A larger grain can accommodate multiple and/or long dislocations such that growth in dislocation density is only limited by the applied stress, not the grain’s size. In contrast, dislocation multiplication in smaller grains is suppressed due to the large stress needed to bend and elongate a short dislocation confined to a small grain size. One may therefore expect a decrease in dislocation density when the grains shrink below a certain size. In addition, dislocation multiplication implies that a significant portion of strain is accommodated by dislocation creep. However, as the grains shrink to sizes where dislocation creep is no longer the primary creep mechanism, one may expect the processes responsible for nucleating and elongating the dislocations to be less efficient and thus for the dislocation density to decrease.

In the limit when the grains are large and the material deforms predominantly by dislocation creep, we assume that dislocation dynamics is independent of grain size and that the steady-state dislocation density (denoted by $\omega_0$ for this limiting case) depends solely on stress; this is consistent with experimental observations, as well as theoretical considerations of the balance between the applied stress and the stress around a dislocation, which suggest the following correlation between deviatoric stress and dislocation density (Twiss 1977; Kohlstedt & Weathers 1980):

$$\omega_0 = \left( \frac{\tau}{Gb} \right)^2, \quad (10)$$

where $\tau^2$ is the grain-specific [through $\mathbf{C}$, see eq. (5)] second invariant of deviatoric stress acting on the grain. To account for the decrease in dislocation density for smaller grain sizes, we propose an additional grain size dependent factor:

$$f(R) = \left( \frac{R/R_c}{1 + R/R_c} \right)^2, \quad (11)$$

where $R_c$ defines the grain size below which the dislocation density becomes grain size sensitive, that is, $f(R) \rightarrow 1$ for $R >> R_c$ and $f(R) \rightarrow 0$ for $R << R_c$. If, for example, the decrease in dislocation density is due to the inefficiency of the Frank-Read sources, then $R_c$ can be approximated using the expression for the stress required to bend a dislocation. Specifically, assuming that the maximum dislocation length is proportional to grain size, then the critical grain size at which dislocation multiplication by Frank–Read sources is possible at a given stress $\tau$ is:

$$R_{FR} = \frac{Gb}{\tau}, \quad (12)$$

where we used (9) with $L = R_{FR}$ and $C_{FR} = 1$. Alternatively, if dislocation density decreases due to the grains shrinking and crossing into a deformation regime where dislocation creep is no longer
dominant, then $\dot{R}$ can be approximated by the field boundary grain size $\dot{R}_F$. For simplicity, we assume that there are only two possible mechanisms by which the material can deform: diffusion and dislocation creep. The strain rate is given by a linear superposition of mechanisms by which the material can deform: diffusion and dislocation creep rheologies (see Table 1). Grains deform predominantly by dislocation creep when $R > \dot{R}_F$, and by diffusion creep when $R < \dot{R}_F$. Regardless of whether we choose to use eqs (12) or (13) as our expression for $\dot{R}$, they yield a similar dependence of $\dot{R}$ on stress to the power of approximately $-1$ (using values for $n$ and $m$ that are typical for olivine, see Table 1). However, $\dot{R}_F$ is strongly temperature-dependent (through the rheological compliances $A_R$ and $B_R$, see Table 1), whereas $\dot{R}_{RF}$ is only weakly temperature-dependent (through the shear modulus $G$, which changes from 70 to 65 as the temperature increases from 1000 K to 1400 K, see Isaak (1992)). To exemplify, at a temperature of 1000 K, as $\tau$ increases from 1 to 100 MPa, $\dot{R}_F$ decreases from 500 to 10 $\mu$m, while $\dot{R}_{RF}$ decreases from 35 to 0.35 $\mu$m; for the same stress-range at 1400 K, both $\dot{R}_F$ and $\dot{R}_{RF}$ decrease from 35 to 0.35 $\mu$m.

For the results presented in this paper we will use $\dot{R}_F = \dot{R}_F$, but we note that there is no compelling reason to choosing eqs (12) or (13).

We combine the effect of stress (10) and grain size (11) on the steady-state dislocation density $\dot{\omega}_0$ as following (see also Fig. 1):

$$\dot{\omega}_0 = \dot{\omega}_0 f(\tau) = \left(\frac{C \tau A}{G b \tau} \frac{R / \dot{R}_F}{1 + R / \dot{R}_F}\right)^{1/2}.$$

The ideal experiment to test our assumed relation between the grain size and the dislocation density in (14) would involve formation of a polycrystalline rock that undergoes dynamic recrystallization solely by grain boundary migration. However, in the published experimental studies, recrystallization by subgrain formation also takes place, which is a process not currently featured in our model.

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**Table 1.** Material and model properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value / Definition</th>
<th>Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas constant</td>
<td>$R_G$</td>
<td>8.3144598</td>
<td>J K$^{-1}$ mol$^{-1}$</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>$G$</td>
<td>70</td>
<td>GPa</td>
</tr>
<tr>
<td>Length of Burgers vector</td>
<td>$b$</td>
<td>0.50</td>
<td>nm</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>$\nu$</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>Energy per dislocation length</td>
<td>$\gamma_d$</td>
<td>varied</td>
<td></td>
</tr>
<tr>
<td>Surface tension</td>
<td>$\gamma$</td>
<td>1</td>
<td>Jm$^{-1}$</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T$</td>
<td>1000</td>
<td>K</td>
</tr>
<tr>
<td>Square-root of second invariant of applied deviatoric stress</td>
<td>$\tau_A$</td>
<td>1–100</td>
<td>MPa</td>
</tr>
</tbody>
</table>

**Dislocation creep**

$$\dot{\gamma}_{disl} = A_{\gamma} \tau_A^n$$

**Compliance**

$$C_{disl} = \frac{A_0 \exp \left( \frac{E_{disl}}{RT} \right)}{\tau_A^n}$$

**Activation energy**

$$E_{disl} = 530$$

**Pre-factor**

$$A_0 = 1.1 \times 10^5$$

**Stress exponent**

$n = 3.5$

**Diffusion creep**

$$\dot{\gamma}_{diff} = B_{\gamma} R^{-m} \tau_A$$

**Compliance**

$$C_{diff} = \frac{B_0 \exp \left( \frac{E_{diff}}{RT} \right)}{\tau_A^m}$$

**Activation energy**

$$E_{diff} = 375$$

**Pre-factor**

$$B_0 = 1.5 \times 10^9$$

**Grain size exponent**

$m = 3$

**Grain model scales**

$$R_s = 10^{-3}$$

$$C_0 = \text{varied}$$

$$C_1 = 10^{-17}$$

$$C_2 = 10^{-11}$$

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*Olivine creep laws from Hirth & Kohlstedt (2003). Microscopic rheological compliances are typically inferred from an averaged value measured for an ensemble of grains (see Rozel et al. 2011, section 5.2).*
Experiments do suggest that the small subgrains and recrystallized mineral grains tend to be dislocation-free (Twiss 1977), but it would be hard to distinguish between the newly formed dislocation-free grains, and the shrinking grains which, according to our assumption, would also see a decrease in dislocation density. Thus, while our models predicted grain size and steady-state dislocation density for grains deforming by dislocation creep can be tested against published experimental studies (e.g. Green & Radcliffe 1972; Kohlstedt & Goetze 1974; Goetze 1975; Durham et al. 1977; Goetze & Kohlstedt 1977; Mercier et al. 1977; Twiss 1977; Toriumi 1979; Schmid et al. 1980; Schmid 1982; Bai & Kohlstedt 1992; Kohlstedt & Hansen 2015), it is less so for the assumed relationship in (14).

Bearing in mind the aforementioned complexities and uncertainty related to dislocation dynamics, we use a simple parametrized model for the rate of change of mobile dislocation density \( \dot{\omega} \) for the purpose of our study, which is similar to the models used previously (e.g. Webster 1966; Karato 2008):

\[
\dot{\omega} = C_i \dot{\omega}(\bar{a} - \sqrt{\omega})
\]  

(15)

where \( C_i \) is a constant with dimensions of \( m \ s^{-1} \), and

\[
\bar{a} = \sqrt{\omega} \equiv \frac{C_i \tau_d}{Gb} \frac{R_i/R_p}{1 + R/R_p}.
\]  

(16)

Note that \( \dot{\omega} = 0 \) when \( \bar{a} = \bar{a}^2 \), and thus \( \bar{a} \) determines dislocation density at the steady state.

To explain the main concepts of the theory, and to build physical intuition, we first introduce a toy-model for a system that consists of only two grains. We then present a model that consists of an ensemble of grains, and which can be used to incorporate this microphysical theory into a larger scale continuum mechanical model.

3 A TALE OF TWO GRAINS

To gain intuition for the interaction between the two driving mechanisms (variations in grain boundary curvature and dislocation density) for recrystallization by grain boundary migration, we first consider a system that consists of only two grains. The grains have the same mineralic compositions and deform due to an applied constant stress and their sizes evolve by a continuous diffusive mass exchange (i.e. no grain splitting or coalescence; see Ricard & Bercovici 2009). The grains’ internal energy can be altered by changes in grain boundary surface energy (determined by grain size) and the density of intragranular defects (i.e. dislocations).

3.1 Governing equations

Each grain’s geometry is assumed to be spherical and described by the relations (1)–(3). We use subscript \( i \) with \( i = 1 \) or 2 to refer to individual grains, such that, for example, \( R_i \) and \( R_2 \) refer to the sizes of grains 1 and 2, respectively. Note that whenever a subscript is used to refer to a specific grain property, we drop the ‘breve’ accent. By mass conservation,

\[
R_2 = (V - R_1)^{1/3},
\]  

(17)

where \( V \) is the total volume of the two grains divided by a factor of \( 4\pi/3 \).

Analogous to the physical reasoning put forward in Hillert (1965), we wish to design a model for the rate of change of an individual grain size \( \dot{R} \) with the characteristic feature that it is positive for \( R \) larger than some critical grain size (in the case of two grains, it is the size of the other grain, while in a more general model with many grains it is the average grain size), but negative otherwise. In addition, we wish for \( R \) to be positive for \( \omega \) smaller than some critical dislocation density (for the two grain model, it is the dislocation density of the other grain, while in many-grains model it is the average dislocation density), but negative otherwise. For the two-grain model, we propose the following expression for the rate of change of grain size, driven by variations in grain size (or rather grain boundary curvature) and dislocation density (see Section 4.3.4, and in particular (90), for the more general derivation of the grain size evolution model, based on considerations of energy conservation and entropy positivity):

\[
\dot{R}_i = R_i^{\beta - 2} R_i^p C_i \left[ (R_i^{-1} - R_1^{-1}) + C_1 (\omega_2 - \omega_1) \right],
\]  

(18)

where \( C_0 \) and \( C_1 \) are constants with dimensions of \( m \) and \( m^7 - 2\pi/\lambda \), respectively, and \( p \) can be positive or negative (we generally use \( p = 2 \), which corresponds to normal grain-growth behaviour; see Ricard & Bercovici 2009). The factor \( R_i^{\beta - 2} R_i^p \) on the right-hand side of (18) is the two-grain version of the grain interaction function that ensures entropy positivity, which we explain in Section 4.3.5. Incorporating grain-specific properties via the subscript \( i \) into (15), the rate of change of dislocation density is given by

\[
\dot{\omega}_i = C_i \omega_i (\bar{a} - \sqrt{\omega}_i)
\]  

(19)

The stress-controlled part of the steady-state dislocation density, \( \omega_{st} \), is given by (10), where we used \( \tau_i = C_i \tau_d \) for the second invariant of stress resolved onto each grain.

We non-dimensionalize (18)–(20) using the following scaling quantities:

\[
R_i \equiv \left( \frac{V}{2} \right)^{1/3}
\]  

(21)

\[
t_i \equiv \frac{R_i^{7-2p}}{C_i}
\]  

(22)

\[
\omega_{st} \equiv 2 \frac{R_i}{R_i^p}
\]  

(23)

such that \( R_i = R_i R_i, R_{si} = R_i R_i \), \( t_i = t_i, \omega_i = a_0, \omega_{st} = a_0 \omega_{st} \), and \( \bar{a}_i = \sqrt{\omega_i/(\omega_i - \omega)} \).

Note that we only need to track size-evolution of one of the grains, since the size of the second grain is given by (17), where the dimensionless volume is now \( V = 2 \). The dimensionless version of eqs (18)–(20) governing the evolution of grain size and dislocation density for a two-grained system becomes (after dropping the primes):

\[
\dot{R}_i = R_i^{\beta - 2} R_i^p \left[ (R_i^{-1} - R_1^{-1}) + \alpha (\omega_2 - \omega_1) \right]
\]  

(24)

\[
\omega_i = \beta \omega_i (\bar{a}_i - \sqrt{\omega_i})
\]  

(25)

\[
\bar{a}_i \equiv \sqrt{\omega_i/(\omega_i - \omega)}
\]  

(26)

\[
R_2 = (2 - R_3)^{1/3}
\]  

(27)
where
\[ \alpha = \frac{2C_{0}}{R_{0}}, \]
(28)
\[ \beta = C_{2}t_{s} \sqrt{\alpha}. \]
(29)

3.1.1 Equilibrium and stability

We analyse the steady states and their stability for the two-grain model, using perturbation analysis. The system is at steady state when \( R_{1} = 0 \) and \( \phi_{1} = 0 \). If \( R_{1} \) is at steady state, then \( R_{1} \) must necessarily be at steady state as well, by mass conservation (27), and thus it suffices to analyse the equilibrium of only one of the grains. We rewrite:
\[ R_{1} = R_{01} + \epsilon R_{1}' \]
(30)
\[ \omega_{0} = \omega_{01} + \epsilon \omega_{01}' \]
where \( \epsilon \ll 1 \) and \( R_{01} \) and \( \omega_{01} \) are equilibrium grain size and dislocation densities, respectively, whereas the infinitesimal perturbations to these equilibria are time-dependent, such that
\[ \dot{R}_{1} = \epsilon \dot{R}_{1}' \]
(32)
\[ \dot{\omega}_{0} = \epsilon \dot{\omega}_{01}'. \]
(33)

We insert (30)–(33) into (24)–(27), linearize it to \( O(\epsilon^{1}) \), and decouple the zeroth- and the first-order terms. The resulting zeroth-order relations [i.e. \( O(\epsilon^{0}) \)], which determine the equilibrium solutions \( R_{01} \) and \( \omega_{01} \), are:
\[ 0 = (2 - R_{01}^{3})^{-1/3} - R_{01}^{-1} + \alpha(\omega_{01} - \omega_{01}) \]
(34)
\[ 0 = \omega_{01} \left( a_{01} - \sqrt{\omega_{01}} \right) \]
(35)
\[ 0 = \omega_{02} \left( a_{02} - \sqrt{\omega_{02}} \right) \]
(36)
where
\[ a_{01} = \frac{\sqrt{\omega_{01}} R_{01}}{R_{1} + R_{01}} \]
(37)
\[ a_{02} = \frac{\sqrt{\omega_{02}}(2 - R_{01}^{3})^{1/3}}{R_{2} + (2 - R_{01}^{3})^{1/3}}. \]
(38)
The growth rates of the perturbations are given by the first order relations (i.e. \( O(\epsilon^{1}) \)):
\[ \dot{R}_{1}' = \left[ R_{01}^{(4-p)/3} + R_{01}^{(4-p)}(2 - R_{01}^{3})^{p/3} \right] R_{1}' + R_{01}^{p/3}(2 - R_{01}^{3})^{p/3} \alpha(\omega_{01}' - \omega_{01}) \]
(39)
\[ \dot{\omega}_{01}' = \beta \left[ \frac{a_{01} R_{1} \omega_{01}}{R_{01}(R_{1} + R_{01})} R_{1}' + \left( a_{01} - \frac{3}{2} \sqrt{\omega_{01}} \right) \omega_{01}' \right] \]
(40)
\[ \dot{\omega}_{02}' = -\beta \left[ \frac{a_{02} R_{2} \omega_{02}}{R_{02}(R_{2} + R_{02})} R_{2}' + \left( a_{02} - \frac{3}{2} \sqrt{\omega_{02}} \right) \omega_{02}' \right]. \]
(41)

Let us first examine the equilibrium states given by (34)–(36). There are two steady-state solutions for the dislocation density for each grain: \( \omega_{01} = 0 \) and \( \omega_{01} = \omega_{01}^{\alpha} \). Note, however, that the solution \( \omega_{01} = 0 \) is always unstable, since it results in a strictly positive growth rate of the perturbations, given by (40) and (41). Our main interest is in the stable equilibrium solutions, and so we will not consider the null solutions for the dislocation densities any further. It remains to determine the stability of the non-null solutions, which we do next. We use the non-null steady-state solutions for dislocation densities to find the equilibrium grain size \( R_{01} \). Using \( \omega_{01} = a_{01}^{\alpha} \) and (37) and (38), we can rewrite (34) in terms of the \( R_{01} \) only:
\[ 0 = (2 - R_{01}^{3})^{−1/3} - R_{01}^{-1} + \alpha \left( \frac{\sqrt{\omega_{01}}(2 - R_{01}^{3})^{1/3}}{R_{2} + (2 - R_{01}^{3})^{1/3}} \right)^{2} - \left( \frac{\sqrt{\omega_{01}} R_{02}}{R_{1} + R_{01}} \right)^{2}. \]
(42)
The multiple solutions to (42) are found numerically and each is inserted into (39)–(41) to determine their stability. Typically there are at most three possible solutions to (42). The set of coupled first order ordinary differential eqs (39)–(41) can be expressed in matrix notation as
\[ \left[ \begin{array}{c} \dot{R}_{1}' \\ \dot{\omega}_{01}' \\ \dot{\omega}_{02}' \end{array} \right] = \hat{H}(R_{01}, a_{01}, \omega_{01}, \alpha, \beta) \left[ \begin{array}{c} R_{1}' \\ \omega_{01}' \\ \omega_{02}' \end{array} \right] \]
(43)
where \( \hat{H} \) is a \( 3 \times 3 \) matrix. The eigenvalues of \( \hat{H} \) determine whether the perturbations will exponentially decay or grow, and thus whether the equilibrium state is stable or unstable, respectively, and whether the system can oscillate around its steady state. The characteristic equation of \( \hat{H} \) is a third order polynomial, and thus there are three roots, or three eigenvalues, for each set of \( R_{01}, a_{01}, \omega_{01}, \alpha \) and \( \beta \). The equilibrium state is stable if the real part of all of the roots are negative, unstable if the real part of at least one of the roots is positive, and oscillates if the most unstable root has an imaginary component, that is, there are one real and two complex conjugate roots, as permitted in cubic algebraic systems (Fig. 2).

When we neglect the effect of dislocation dynamics on grain growth (\( \alpha = 0 \)), the system is inherently unstable (Fig. 2, left and middle): there exists only one equilibrium state in which the grains are of equal size \( R_{1} = R_{2} = 1 \), and it is unstable. Increasing the value of \( \alpha \) increases the contribution from dislocations to the driving force for grain size evolution, which opposes the driving force associated with the variation in surface tension. At sufficiently large \( \alpha (\alpha > \alpha_{cr}) \), the dislocation driving force offsets that of the surface tension, and stabilizes the equilibrium state (Fig. 2). For a given \( C_{12} \), there exists a critical value of \( \alpha (\alpha = \alpha_{cr}) \) that marks the marginal stability of the solutions for (39)–(41) (Fig. 2, left and middle; Fig. 3, left). Stable steady-state solutions exist only for \( \alpha > \alpha_{cr} \), which is when the forces associated with the intragranular defects are significant enough, relative to those associated with grain boundary curvature, so that the system is able to recover from perturbations and converge to its equilibrium state.

When the stress resolved onto each grain is identical (i.e. \( C_{12} = C_{11} \)), the stable equilibrium grain size is identical as well (\( R_{1} = R_{2} = 1 \), Fig. 2, left). However, when \( C_{12} \neq C_{11} \), the stable equilibrium grain size can be different for different grains (Fig. 2, middle and right). Thus, the variation in crystal lattice orientation between different grains, together with the effect of intragranular defects on grain size evolution (i.e. \( \alpha > \alpha_{cr} \)), allow for the coexistence of different grain sizes at steady state. The larger the difference
between $C_{r1}$ and $C_{r2}$, the larger the difference between the equilibrium grain size of each grain (Fig. 2, right), and the larger the value of $\alpha_{cr}$ that is required for the existence of stable steady-state solutions (Fig. 3, left). This is intuitive, since a larger contrast in grain boundary energy (resulting from a larger difference in equilibrium grain sizes when the difference between $C_{r1}$ and $C_{r2}$ is large) leads to a larger force to drive grain growth, and thus would require a larger force associated with the intragranular defects to offset it.

Changing the value of the applied stress $\tau_A$ affects the steady-state dislocation density, according to (16), and thus also $\alpha_{cr}$. An increase in stress yields a larger steady-state dislocation density (Fig. 1), and therefore a lower value of $\alpha_{cr}$ needed to offset grain growth (Fig. 3, right).

The difference in timescales associated with the rate of change of grain size and that of dislocation density can result in oscillatory solutions. The slower the rate of dislocation kinetics (i.e. the smaller the value of $\beta$), or the larger the force associated with the energy of intragranular defects relative to that of the grain boundary energy (i.e. the larger the value of $\alpha$), the larger the time lag between the grain growth and the evolution of dislocation density, and thus the more likely for the oscillatory solutions to emerge (see example in Section 3.1.2). Specifically, for a given $\beta$, there is a critical value of $\alpha$ ($\alpha = \alpha_{osc}$), such that for $\alpha > \alpha_{osc}$ there exist solutions in the form of damped oscillations (Fig. 4, left). Since the steady-state grain size, and thus the grain boundary energy, depend on stress resolved onto each individual grain (i.e. the difference between $C_{r1}$ and $C_{r2}$), so does the value of $\alpha_{osc}$, which is larger for a larger difference between $C_{r1}$ and $C_{r2}$. The frequency of the oscillations is higher for larger values of $\alpha$, as expected, since the driving forces for grain growth, and thus also the rates of grains and dislocations dynamics, scale with $\alpha$ (Fig. 4, right).

### 3.1.2 Nonlinear examples for the system with two grains

We demonstrate the physical application of the results obtained from the stability analysis in the previous section with some nonlinear examples of the grain size and dislocation density evolution in a two-grain system given by the coupled nonlinear system (24)–(27). When $\alpha = 0$, the variation in surface tension provides the only driving force for grain size evolution, making the larger grain ever larger, and the smaller grain ever smaller, until the smaller grain is entirely consumed by the larger one (Fig. 5, light pink and grey lines). The grain coarsening, driven by the reduction in surface energy, can be offset by accounting for the effect of dislocations, using a larger value for $\alpha$. At sufficiently large $\alpha$, the system eventually converges to a stable steady state with a finite grain size (Fig. 5 dark pink and black lines).

Rapid convergence to steady state occurs for a large $\beta$, such that the dislocation density $\omega_0$ adjusts to a changing grain size nearly instantaneously (Fig. 5, left), that is, $\omega_0$ is always close to its steady-state value (Fig. 5, left, where the solid line closely follows the dashed line). Choosing a lower value for $\beta$ causes more complex...
Figure 4. Left: values of $\alpha_{osc}$ above which the solutions to eqs (39)–(41) can oscillate, as a function of $\beta$. Results for different values of $C_{\tau_2}$ are shown (see the legend). Solid lines indicate cases where the oscillations would exponentially decay, while the dashed lines indicate unstable solutions. Right: oscillation frequency (per dimensionless time unit) of the solutions as functions of $\alpha$ ($\alpha > \alpha_{osc}$). Results for $C_{\tau_2} = 0.9$ and two different values of $\beta$ are shown (see the legend). In all cases, $C_{\tau_1} = 1$ and $\tau_A = 1$ MPa.

Figure 5. Evolution of dislocation density $\omega$ (left) and grain size $R$ (right) for a system of two grains (pink lines for $R_1$ and black lines for $R_2$). Accounting for the contribution to grains internal energy from intragranular defects (i.e. dislocations) can offset the coarsening rate, and allow for a stable steady-state grain size (dark pink and black lines, $\alpha = 2.6 \times 10^{-2}$, $C_{\tau_1} = 1$, $C_{\tau_2} = 0.9$, $\beta = 4.2$), as opposed to a runaway grain growth when surface tension is the only driving force (light pink and grey lines, $\alpha = 0$). Dashed lines in the $\omega$-plot are the instantaneous response (i.e. for $\beta \to \infty$) of the dislocation density to the changing grain size. Dashed lines in the $R$-plot are the stable steady-state solutions computed for $\dot{\omega} = 0$ and $\dot{R} = 0$.

4. Behaviour to emerge (Fig. 6), and in particular, both the grain size and the dislocation density oscillate as they approach their steady-state values (as predicted by the linear analysis). Oscillations occur because the dislocation density in a growing grain increases too slowly to offset the force associated with the grain boundary energy, such that the grain size overshoots its steady-state value (Fig. 6). The grain starts shrinking only when the force associated with the intragranular defects has had time to build up and offset grain growth, which is controlled by $\beta$. The cycle repeats again, as the shrinking grain undershoots its steady-state value due to the excessively large dislocation density that is slowly recovering from the preceding overshoot. If the overshoots are not too high (i.e. $\beta$ is sufficiently large to allow for the dislocation density to build up; see Fig. 4, left, where the solid lines indicate stable solutions for sufficiently large $\beta$-values), the oscillations will get damped as the system converges towards a stable steady state.

We can make the following inferences from the simple two-grain model. First, dislocation dynamics can provide a driving mechanism for grain boundary migration that opposes the forces associated with grain boundary surface tension, thus stabilizing grain growth and allowing for finite grain size distributions to exist. Second, the equilibrium grain size can vary between different grains due to the variation in the grains crystal lattice orientation and the resulting stress resolved onto each grain. Finally, the rate at which the system advances towards its steady state is controlled both by the kinetics of diffusion (which controls grain growth), as well as the kinetics of dislocation motion. The competition between the two timescales can lead to oscillatory behaviour.

4. A Tale of Many Grains

We now consider our model system, but for the more general case of an ensemble of grains, rather than just two grains. The physical model builds on the continuum theory of grain size evolution and damage of Ricard & Bercovici (2009), with the main modification being that we now include the contribution from intragranular defects (i.e. dislocations) to the energy and entropy budgets. In the following, we briefly outline the theory of grain size evolution, closely following Ricard & Bercovici (2009), in order to introduce new features and processes.
4.1 Grain size distribution

The sizes of all the grains contained in a volume \( V \) are described by a continuous grain size distribution function \( v_R \), such that the number of grains between sizes \( R \) and \( R + dR \) per volume is \( dn = v_R dR \), where \( v_R \) is a function of position, time and \( R \), and has the units of \( m^{-4} \). Assuming that the grains fill the entire space in the volume \( dV \), such that the sum of all grain volumes equals \( dV \), we get the normalization relation:

\[
\int_0^\infty v_R dR = 1. \tag{44}
\]

Using (44), we can define the volume average of a granular quantity \( \bar{\theta} \) as

\[
\bar{\theta} = \int_0^\infty \theta v_R dR. \tag{45}
\]

The evolution or conservation law for the grain size distribution within a control volume, assuming that material can only be transferred between grains by continuous diffusive processes (i.e. no grain splitting or coalescence), is given by

\[
\frac{\partial v_R}{\partial t} + \nabla \cdot (v_R \nabla \bar{\theta}) + \frac{\partial}{\partial R} (Rv_R) = 0, \tag{46}
\]

where \( v \) is the macroscopic (or bulk material) velocity and \( \bar{\theta} \) is the rate of change of grain size.

The full time derivative \( d/dt \) for physical properties that can vary in space, time and the grain size space is given by

\[
\frac{d}{dt} = \frac{D}{Dt} + \frac{\partial}{\partial R}, \tag{47}
\]

where \( D/Dt \) is the material (or Lagrangian) derivative. Using (46), we can express the rate of change of a granular quantity \( \bar{\theta} \) in a closed and deformable volume \( \delta V \) as

\[
\frac{D\bar{\theta}}{Dt} = \int_{3V} \int_0^\infty \left( \frac{\partial \bar{\theta} v_R}{\partial t} + \nabla \cdot (\bar{\theta} \nabla v_R) \right) dRdV, \tag{48}
\]

where \( \bar{\theta} \) is the total amount of \( \bar{\theta} \) in all grains and in a finite volume \( \delta V \). We assume that \( v_R \to 0 \) as \( R \to 0 \) and \( R \to \delta V^{1/3} \), such that the fluxes of physical quantities through the distribution tails are zero (Ricard & Bercovici 2009, section 2.5). Using (46) and (47), we can rewrite (48) as

\[
\frac{D\bar{\theta}}{Dt} = \int_{3V} \int_0^\infty \frac{d\bar{\theta}}{dt} v_R dRdV. \tag{49}
\]

The mass conservation law for continuous mass exchange between grain populations becomes

\[
\frac{DM}{Dt} = \int_3 \int_0^\infty \frac{d\bar{m}}{dt} v_R dRdV = 0. \tag{50}
\]

where \( M \) is the total mass of \( \delta V \).

4.2 Grain size evolution in an ensemble of grains

In the general model with many grains, we assume that for a given point in space and time, there is a unique value of \( \bar{L} \) associated with a given grain size \( R \). This is a simplification, since, generally speaking, grains of equal size can have independent numbers of dislocations. However, accounting for different dislocation densities of each individual grain quickly becomes excessively mathematically cumbersome, because it adds another independent dimension to the grain size distribution. Our simplifying assumption is valid if we assume that the dislocation density in each grain is always close to its steady-state value \( \bar{\omega}_0 = \bar{\omega}_0 \), determined by the stress and the grain size (16), and that there is small variation in \( \bar{C}_r \) between different grains. Experimental studies show that the steady-state dislocation density is reached at relatively low strains (i.e. \( < 2 \) per cent (Durham et al. 1977)). Thus, it is reasonable to assume that, at least for some deformation conditions, the timescale at which the dislocation density reaches its steady state is much shorter than that for diffusive grain growth, such that \( \bar{\omega} \) is close to \( \bar{\omega}_0 \).

During a time interval \( dt \), the total length of dislocations within a grain changes along with the changing grain size, as dislocation density adjusts to its grain size-specific steady-state value. An incremental change in total length of dislocations is given by

\[
\frac{d\bar{L}}{dt} = \bar{\omega} d\bar{V}. \tag{51}
\]

4.3 Conservation laws

4.3.1 Force balance

Within the limiting assumptions that factor \( \bar{C}_r \) (5) is the same for all of the grains in our model, and that the dislocation density is only a function of stress and grain size, all grains of the same radius experience the same full stress and strain rate tensors \( \bar{\sigma} \) and \( \bar{\epsilon} \), respectively. The volume averaged (i.e. averaged over all grain sizes) stress and strain rate can thus be defined according to (45)
as:
\[
\sigma = \int_0^\infty \tilde{\sigma} \nu \eta \, d\tilde{R}
\]
(52)
\[
\dot{\tilde{\epsilon}} = \int_0^\infty \tilde{\eta} \nu \eta \, d\tilde{R}.
\]
(53)
The volume-averaged stress can be decomposed into the averaged pressure and deviatoric stress, as following:
\[
\sigma = -P \mathbf{I} + \tilde{\sigma}
\]
(54)
where \( \mathbf{I} \) is the identity matrix.

Forces acting on a control volume \( \delta V \) are the body forces:
\[
F_b = \int_{\delta V} \rho g \nu \eta \, dV,
\]
(55)
here the only body force is due to \( g \), the gravitational acceleration.

The surface forces due to an applied stress are (Ricard & Bercovici 2009, section 2.4):
\[
F_s = \int_{\partial V} \nabla \cdot \sigma \nu \eta \, d\mathcal{A}.
\]
(56)
The line forces due to surface tension acting on the grains that are cut by the surface \( \delta A \) are (Bercovici et al. 2001, appendix A):
\[
F_l = \int_{\delta A} \nabla (\gamma K) \nu \eta \, d\mathcal{A},
\]
(57)
where \( \gamma \) is the surface tension and \( K \) is the volume-averaged grain boundary curvature, defined using (3) and (45) as
\[
K = \int_0^\infty \tilde{K} \nu \eta \, d\tilde{R}.
\]
(58)
The balance of forces acting on an arbitrary volume within the grained medium is given by
\[
\rho g + \nabla \cdot \sigma + \nabla (\gamma K) = 0.
\]
(59)

4.3.2 Energy balance

The total intrinsic energy in a volume \( \delta V \) is made up of the volumetric internal energy, total surface grain boundary energy, and the energy associated with intragranular defects (i.e., dislocations):
\[
E = \int_{\delta V} \int_0^\infty (\tilde{\epsilon} \rho \tilde{s} + \gamma \tilde{A} + \gamma_d \tilde{L}) \nu \zeta \eta \, d\mathcal{A} \, d\tilde{R} \, dV.
\]
(60)
The rate of change of total energy is thus
\[
\frac{DE}{dt} = \int_{\delta V} \int_0^\infty \left( \tilde{m} \frac{d\tilde{s}}{dt} + \gamma \tilde{A} + \gamma_d \tilde{L} \right) \nu \zeta \eta \, d\mathcal{A} \, d\tilde{R} \, dV.
\]
(61)

The rate of change of an increment of total energy \( E \) can also be expressed in terms of a grains entropy (\( \tilde{S} = \tilde{m} \tilde{s} \)), pressure (\( \tilde{P} \)) and chemical potential (\( \tilde{\mu} \)), using a Gibbs relation. Assuming that the temperature \( T \) in the volume \( \delta V \) is uniform and ignoring the contribution from elastic strain energy (i.e. the elastic strain energy is assumed to build up and get released on a much shorter timescale than the processes involved in viscous deformation, which are the focus here), we get:
\[
\frac{DE}{dt} = \int_{\delta V} \int_0^\infty \left( \tilde{m} \frac{d\tilde{s}}{dt} - \tilde{P} \frac{d\tilde{m}}{\rho} \frac{1}{\rho} \frac{1}{dt} \right) + \tilde{\mu} \frac{d\tilde{m}}{dt} + \gamma \tilde{A} + \gamma_d \tilde{L} \right) \nu \zeta \eta \, d\mathcal{A} \, d\tilde{R} \, dV,
\]
(62)
where we also used the relation for grain volume \( \nu = \tilde{m} / \rho \). Equating (61) and (62) yields:
\[
0 = \int_{\delta V} \int_0^\infty \left[ \tilde{m} \left( \frac{d\tilde{s}}{dt} - \tilde{T} \frac{d\tilde{L}}{dt} + \tilde{P} \frac{d(1/\rho)}{dt} \right) + \tilde{\mu} \frac{d\tilde{m}}{dt} \right] \nu \zeta \eta \, d\mathcal{A} \, d\tilde{R} \, dV.
\]
(63)
Eq. (63) holds for any grain size distribution and kinetic law if we require that the internal energy goes as:
\[
d\tilde{s} = T d\tilde{s} - \tilde{P} d(1/\rho),
\]
(64)
as well as that the term \( (\tilde{\epsilon} - \tilde{T} \tilde{s} + \tilde{\mu} / \tilde{\rho}) \), which represents the background energy state, is at most a constant independent of \( R \).

Adopting the definition:
\[
\tilde{\mu} = \tilde{\epsilon} - \tilde{T} \tilde{s} + \frac{\tilde{\mu}}{\tilde{\rho}},
\]
(65)
and assuming incompressibility (which yields \( d\tilde{s} = T d\tilde{s} \), or \( \tilde{\epsilon} = \tilde{T} \tilde{s} \) by expansion of scales), we get that the chemical potential for our system is given by
\[
\tilde{\mu} = \frac{\tilde{P}}{\tilde{\rho}}.
\]
(66)

We consider the rate of change of total energy in a fixed and open volume \( \delta V \) bounded by the surface area \( \delta A \), as dictated by the energy fluxes \( J \), mechanical work \( W \) done on the volume and internal heat production \( Q \). The flux of energy associated with the mass transport at velocity \( \nu \) is given by (Ricard & Bercovici 2009, section 4.2.1):
\[
J_k = \int_{\delta A} \int_0^\infty (\tilde{m} \tilde{\epsilon} + \gamma \tilde{A} + \gamma_d \tilde{L}) \nu \zeta \eta \, d\mathcal{A} \, d\tilde{R} \, d\mathcal{A},
\]
(67)
where \( \tilde{h} \) is the unit vector normal to \( \delta A \). The three terms inside the integral represent the flux of internal energy due to mass transport \( (\tilde{m} \tilde{\epsilon}) \), the flux of surface energy associated with grain boundary energy \( (\gamma \tilde{A}) \), and the flux of energy associated with dislocations. Dislocations can contribute to the energy budget of a control volume in three ways. First, when a grain containing dislocations enters a control volume, it brings the energy associated with the dislocations into the volume. This energy flux is associated with the bulk motion of the grained material, and is represented by the third term of the sum in (67). Second, dislocations can move through the grains independently of the bulk material motion, and thus move into and out of the control volume if they happen to be inside the grains that are cut by the area element \( \delta A \). Since we assume that the dislocation density is homogeneous within the grain, and that the motion of the dislocations accommodating deformation can be along all possible planes and directions, there is no preferred net dislocation motion across a grain, and thus no net contribution to the energy flux. Third, there is a force acting on a dislocation due to the presence of ambient stress, so that the motion of a dislocation that is cut by the surface \( \delta A \) does work on that surface. However, since this contribution to mechanical work arises exclusively due to the presence of ambient stress, it is already accounted for by the net work done on \( \delta V \) (68), which we discuss next.
The body, surface and line forces (eqs 55–57) acting on the volume $dV$ sum up to the following rate of mechanical work, respectively (Ricard & Bercovici 2009, section 4.2.2),

$$ W = \int_0^\infty \int_0^\infty \hat{n} \cdot \mathbf{v} \mathbf{v} \cdot dR dV $$

$$ + \int_0^\infty \int_0^\infty \hat{\nu} \cdot \hat{\nu} \mathbf{v} \mathbf{v} \cdot dR dA $$

$$ + \int_0^\infty \int_0^\infty \gamma \hat{\mathbf{K}} \cdot \hat{n} \mathbf{v} \mathbf{v} \cdot dR dA. $$

Using the divergence theorem to express (67) and (68) as volume integrals and noting that these relations must hold for an arbitrary volume (i.e. we can eliminate the volume integral), we arrive at the following energy conservation relation:

$$ \frac{\partial E}{\partial t} = \int_0^\infty \left( \frac{\partial (\hat{m} \mathbf{v} \mathbf{v})}{\partial t} + \gamma (\hat{A} \mathbf{v} \mathbf{v}) + \gamma (\hat{L} \mathbf{v} \mathbf{v}) \right) dR $$

$$ = \int_0^\infty -\nabla \cdot \left( (\hat{m} \mathbf{v} \mathbf{v} + \gamma \hat{A} \mathbf{v} \mathbf{v} + \gamma \hat{L} \mathbf{v} \mathbf{v}) \right) dR $$

$$ + \int_0^\infty \hat{m} \mathbf{v} \mathbf{v} dR $$

$$ + \int_0^\infty \mathbf{v} \cdot \left( \nabla \left[ (\hat{\nu} \mathbf{v} \mathbf{v} + \gamma \hat{K} \mathbf{v} \mathbf{v} \right) \right] dR - \nabla \cdot \mathbf{q} + Q. $$

(69)

where $\mathbf{q}$ is the heat flux vector, assumed to be grain size independent. Using $\mathbf{\tau}$ the force balance (59) and assuming incompressibility (i.e. $\nabla \cdot \mathbf{v} = 0$), we can rewrite (69) as:

$$ \int_0^\infty \left( \frac{d(\hat{m} \mathbf{v} \mathbf{v})}{dt} + \frac{d(\hat{\nu} \mathbf{v} \mathbf{v})}{dt} + \frac{d(\gamma \hat{L} \mathbf{v} \mathbf{v})}{dt} \right) dR = \Psi - \nabla \cdot \mathbf{q} + Q $$

(70)

where we also used (49) to express the rate of change of a granular quantity in a deforming volume, and where $\Psi = \nabla \cdot \mathbf{\tau} \cdot \mathbf{\varepsilon}$ is the rate of deformational work and $\mathbf{\tau}$ and $\mathbf{\varepsilon}$ are the grain size averaged deviatoric part of the stress tensor and strain rate, respectively.

### 4.3.3 Entropy production

Next, we find the relation that guarantees that the second law of thermodynamics in a volume $dV$ is satisfied, which states that the internal entropy production in a volume $dV$ is necessarily greater than zero. The rate of change of internal entropy in a deforming volume $dV$ is (Ricard & Bercovici 2009, section 4.3):

$$ \frac{DS}{dt} + \int_{\delta d} \mathbf{j}_s \cdot \hat{n} dA = \int_0^\infty \int_0^\infty \frac{d(\hat{m} \mathbf{v} \mathbf{v})}{dt} + \nabla \cdot \left( \frac{\mathbf{q}}{T} \right) \geq 0, $$

(71)

where $\mathbf{j}_s = \mathbf{q} / T$ is the entropy flux through the volume’s surface $\delta d$, which we assume is due to heat flux. Using (64) and (65), we can express the full time derivative of granular internal energy as:

$$ \frac{d}{dt} (\hat{m} \mathbf{v} \mathbf{v}) = \hat{\mu} \frac{d\hat{m}}{dt} + T (\frac{d(\hat{m} \mathbf{v} \mathbf{v})}{dt} + \frac{d(\hat{\nu} \mathbf{v} \mathbf{v})}{dt} - \hat{P} \frac{d\mathbf{v}}{dt}. $$

(72)

Inserting (72) into the energy conservation law (70), we can substitute the resulting relation for the grain specific entropy in (71), to arrive at the following condition for entropy positivity:

$$ \int_0^\infty \left( \hat{P} \frac{d\mathbf{v}}{dt} - \hat{\mu} \frac{d\hat{m}}{dt} - \gamma \frac{d\mathbf{A}}{dt} - \gamma \frac{d\hat{L}}{dt} \right) \mathbf{v} \mathbf{v} dR $$

$$ + \Psi - \frac{1}{T} \mathbf{\nabla} \cdot \mathbf{\nabla} + Q \geq 0. $$

(73)

Eq. (73) can be further simplified if we assume that the material is incompressible (such that, according to (66), $\hat{\mu} \frac{d\hat{m}}{dt} = \hat{P} \frac{d\mathbf{v}}{dt}$), and that by Curies principle, the integral over the scalar products in the first term in (73) and the higher rank tensorial products must satisfy the inequality independently. Thus, the entropy positivity relation that is directly related to the energy of the grain boundaries and intragranular defects becomes [using (3) and (51)]:

$$ \int_0^\infty \left( \gamma \hat{K} + \gamma_\varepsilon \hat{\omega} \right) \frac{d\hat{m}}{dt} \mathbf{v} \mathbf{v} dR \geq 0. $$

(74)

### 4.3.4 Grain interaction

The terms $\gamma \hat{K}$ and $\gamma_\varepsilon \hat{\omega}$ constitute the ‘thermodynamic forces’ that induce mass-transfer across grain populations (say, from grains of size $R$ to grains of size $R'$) in our system. We assume that the thermodynamic forces and fluxes are linearly coupled, as following:

$$ \frac{d\hat{m}(R)}{dt} = \int_0^\infty G^I(R, R') \left( \gamma \hat{K}(R') + \gamma_\varepsilon \hat{\omega}(R') \right) \mathbf{v} \mathbf{v} dR' $$

(75)

where $G^I(R, R')$ is the grain interaction function, to be specified, that relates the free energies of grains of size $R$ to the growth of grains of size $R$. Invoking Onsager’s reciprocal relation, we require for $G^I(R, R')$ to be symmetric:

$$ G^I(R, R') = G^I(R', R), $$

(76)

and, in order to satisfy mass conservation for any grain size distribution, Ricard & Bercovici (2009, see eq. (76)) show that:

$$ \int_0^\infty G^I(R, R') \mathbf{v} \mathbf{v} dR = \int_0^\infty G^I(R', R) \mathbf{v} \mathbf{v} dR = 0. $$

(77)

For brevity of notation, let us introduce $dn = \mathbf{v} \mathbf{v} dR$, $dn' = \mathbf{v} \mathbf{v} dR'$, $\mathbf{K}(R) = \mathbf{K}$, $\mathbf{K}(R') = \mathbf{K}'$, $\hat{\omega}(R) = \hat{\omega}$, and $\hat{\omega}(R') = \hat{\omega}'$. The equality in (77) allows us to rewrite the expression for the rate of mass transfer from grains of size $R$ in terms of their difference in grain boundary curvature and dislocation density from the other grains:

$$ \frac{d\hat{m}(R)}{dt} = \int_0^\infty G^I(R, R') \left[ \gamma (\mathbf{K}' - \mathbf{K}) + \gamma_\varepsilon (\hat{\omega}' - \hat{\omega}) \right] dn' $$

(78)

and,

$$ \int_0^\infty G^I(R, R') \left[ \gamma (\mathbf{K}' - \mathbf{K}) + \gamma_\varepsilon (\hat{\omega}' - \hat{\omega}) \right] dn = 0. $$

(79)

We can express the coarsening dissipation rate, which enters the entropy positivity relation (74), as following:

$$ -\int_0^\infty \left( \frac{d\hat{m}(R)}{dt} \left[ \gamma \hat{K} + \gamma_\varepsilon \hat{\omega} \right] \mathbf{v} \mathbf{v} dR \right) $$

(80)

$$ = -\int_0^\infty \int_0^\infty G^I(R, R') \left[ \gamma (\mathbf{K}' - \mathbf{K}) + \gamma_\varepsilon (\hat{\omega}' - \hat{\omega}) \right] $$

$$ \times (\gamma \hat{K} + \gamma_\varepsilon \hat{\omega}) dn' dn $$

$$ = -\int_0^\infty \int_0^\infty G^F(R', R) \left[ \gamma (\mathbf{K}' - \mathbf{K}) + \gamma_\varepsilon (\hat{\omega}' - \hat{\omega}) \right] $$

$$ \times (\gamma \hat{K}' + \gamma_\varepsilon \hat{\omega}') dn' dn', $$

since the double integrals on the right are invariant to an interchange of the integration variables $R$ and $R'$. The symmetry of $G^I(R, R')$ by
The entropy positivity relation (74) requires \( G(R, R') \) to be a positive function. As an example (which we will adopt for the rest of this paper), a quadratic product between functions of \( R \) and \( R' \) would yield a \( G(R, R') \) that satisfies all of the above constraints (i.e., Eqs. 76 and 77 and \( G(R, R') > 0 \)).

\[
G(R, R') = B(R)B(R').
\]

Using (82), the rate of mass transfer from the grains of size \( R \) according to (78) can be rewritten as

\[
\frac{\mathrm{d}n(R)}{\mathrm{d}t} = B(R)\int_0^\infty B(R')\left[\gamma(\tilde{K}' - \tilde{K}) + \gamma_4(\tilde{\omega}' - \tilde{\omega})\right] \mathrm{d}n'.
\]

Defining an average weighted by \( B(R) \) of a granular quantity \( \tilde{\theta} \) as

\[
\overline{\theta} = \frac{\int_0^\infty \theta B(R)v_{\theta} dR}{\int_0^\infty B(R)v_{\theta} dR}
\]

and defining

\[
\beta(R) = B(R)\int_0^\infty B(R')v_{\theta} dR',
\]

we finally arrive at the following expression for the rate mass transfer from grains of size \( R \):

\[
\frac{\mathrm{d}n(R)}{\mathrm{d}t} = \beta(R)\left[\gamma(\tilde{K}' - \tilde{K}(R)) + \gamma_4(\tilde{\omega}' - \tilde{\omega}(R))\right].
\]

We choose a simple power-law relation for \( B(R) \) [see Ricard & Bercovici (2009, section 5.2)], which satisfies the power-law relation for grain growth, consistent with experimental and theoretical studies (Lifshitz & Slyozov 1961; Hillert 1965):

\[
B(R) = \sqrt{4\pi \rho \theta^3 R^p},
\]

which leads to:

\[
\beta(R) = 4\pi \rho \theta^3 I_p R^p,
\]

where \( \theta^3 \) is a constant with dimensions \( \text{m}^2 \cdot \text{kg}^{-1} \cdot \text{s} \), and where

\[
I_p = \int_0^\infty R^p v_{\theta} dR.
\]

Using (3) and (4) with (86), the rate of grain size change, driven by variations in grain boundary curvature and dislocation density, is given by

\[
\dot{R} = C_1 I_p R^{p-2}\left[\left(R^{-1}_1 - R^{-1}ight) + \frac{\gamma_4}{2\gamma}(\tilde{\omega} - \tilde{\omega})\right]
\]

where

\[
C_1 = 2\gamma B_0^3.
\]

We next non-dimensionalize our system of equations, using a length scale \( R_e \) (see Table 1), as well as (22) and (23) for time and dislocation density scales. In addition, we define \( I_p = R_e^{p-3} I_p \) and \( v_R = R_e^{-3} v' \). The dimensionless set of equations governing the evolution of grain size becomes (after dropping the primes):

\[
\dot{R} = I_p R^{p-2}\left[\left(R^{-1}_1 - R^{-1}\right) + \alpha(\bar{\omega} - \bar{\omega})\right]
\]

\[
\frac{\mathrm{D}v_R}{\mathrm{D}t} + \frac{\partial}{\partial R}(Rv_R) = 0
\]

which includes the evolution law for grain size distribution (46) and where \( \alpha \) is given by

\[
\alpha = \frac{\gamma_4}{R_e\gamma}.
\]

Dislocation density changes along with the changing grain size and, assuming that it adjusts instantaneously to its equilibrium value (note that this is different from the two-grain model, where \( \omega \) could evolve towards its equilibrium state at a rate governed by \( \beta \)), is given by

\[
\bar{\omega} = \bar{\omega}_R
\]

\[
\bar{\omega} = \sqrt{\omega / R_e} / (\gamma R_e).
\]

Since we assumed that \( \bar{C}_1 \) is uniform for all the grains, it follows that \( \bar{\omega}_R \) is also identical for all the grains.

### 4.3.5 Flashback to the two-grain model

The grain size evolution equation for the two grain system (24) can be deduced from that of the general model (92), which we herein demonstrate. The grain size distribution function for the system of two grains has the following form:

\[
v_R = \left(\frac{1}{(4/3)\pi F}\right)\left[\delta(R - R_1) + \delta(R - R_2)\right].
\]

where \( \delta \) is the Dirac-Delta function, which obeys the following integration equality:

\[
\int_a^b f(R)\delta(R - R^*) \mathrm{d}R = \begin{cases} f(R^*), & \text{if } a < R^* < b \\ 0, & \text{otherwise} \end{cases}
\]

Using eq. (97) and Section 97.5, the average of a granular property \( \overline{\theta} \) (84), weighted by the function \( B(R) \) (87) that defines the grain interaction function (82) becomes:

\[
\overline{\theta} = \theta_1 R_1^p + \theta_2 R_2^p R_e^{p-3} + \frac{\theta_3}{R_e^p + R_e^p R_e^{p-3}}.
\]

Using (98) to determine the averaged properties and \( I_p \) in the general grain size evolution eq. (92) yields (24), which is the rate of grain growth for the two grain system.

## 5 Examples for the system with many grains

Given the limitations of the general model with a large number of grains (the dislocation density \( \omega \) is always at steady state and the factor \( \bar{C}_1 \) is the same for all of the grains), we cannot test the effects of varying \( \beta \) and \( \bar{C}_1 \), as we did for the simple two-grain model in Section 3. However, the prediction based on the results from the two-grain model that the presence of intragranular defects (dislocations) can offset coarsening and result in a finite steady-state
grain size can still be tested for a system with a large number of grains. We consider a model with an arbitrarily large number of grains, whose initial grain size distribution is given by

\[ v_g = \frac{1}{\sqrt{2\pi C_3}} \exp\left[ -\frac{(R - R_c)^2}{2C_3^2} \right]. \]  \quad (99)

where \( C_3 \) is the standard deviation and \( R_c \) is the mean grain size. The evolution of grain size and dislocation density for this system is described by (92)-(93).

As a reference case, we first consider the grain coarsening model with \( \alpha = 0 \) (i.e. without the effect of dislocation dynamics) (Fig. 7, top row). The larger grains grow at the cost of the smaller grains and, since the smaller grains shrink faster than the larger grains grow (Fig. 7, top left plot), the grain size distribution broadens and its peak shifts towards larger grain sizes (Fig. 7, top right plot). The associated increase in the mean grain size and variance (Fig. 8, dotted line) are a typical feature of normal grain growth (Hillert 1965).

Increasing the contribution from dislocations to the grains internal energy (i.e. increasing the value of \( \alpha \)) decreases the rate at which the larger grains grow (Fig. 7, middle row, left), since the decrease in grain boundary energy (i.e. loss of small grains into the bigger grains) now comes at the price of increasing dislocation energy, both of which affect grain growth. The result is a strongly suppressed coarsening rate, with little change in mean grain size and variance through time (Fig. 8, dashed line). This case is similar to the marginally stable cases with \( \alpha \) that, depending on the value chosen for \( \alpha \) and dislocation density). Specifically, there exists a critical value for \( \alpha \) (\( \alpha = \alpha_{cr} \)), such that when \( \alpha > \alpha_{cr} \) the system can reach a stable equilibrium. In the more general model with many grains, albeit with the simplifying assumptions of homogeneous stress and a dislocation density that depends instantaneously on grain size, we demonstrated in Section 5 that, analogous to the two-grain model, the value of \( \alpha \) determines the fate of the grain size distribution. In particular, the system undergoes normal coarsening when \( \alpha \) is small, with the coarsening rate being suppressed for higher values of \( \alpha \), and, finally, the system tends towards a finite steady-state grain size for sufficiently large values of \( \alpha \). The two-grain and the many-grains model thus both infer that accounting for the grains internal energy contribution from intragranular defects (i.e. having a sufficiently large \( \alpha \)) stabilizes grain growth and allows for a finite steady-state grain size.

It is interesting to see what this result means for the physical properties of rocks. The parameter \( \alpha \) (94) is the ratio between energies associated with the grain boundaries \( \gamma \) and the intragranular defects \( \gamma_d \), scaled by a reference grain size \( R_c \) (see Table 1). For an applied stress of \( \tau_d = 1 \text{ MPa} \) (assumed homogeneous here, i.e. \( C_t = 1 \)), the two-grain model predicts \( \alpha_{cr} \) on the order of \( 10^{-2} \) (Figs 2 and 3, right). An analogous case of \( \alpha_{cr} \) for the many-grains model would be a grain size distribution with a mean grain size and variance that remain more or less constant through time—that is, a value for \( \alpha \) at which the system neither coarsens nor converges to a single grain size. This is similar to the case with \( \alpha = 3.5 \times 10^{-3} \) in the many-grains model (Fig. 7, middle row). Using the values from Table 1 for \( \gamma \) and \( R_c \), for \( 10^{-3} < \alpha_{cr} < 10^{-2} \) (which spans the range of \( \alpha_{cr} \) for the two-grain and the many-grains models with \( \tau_d = 1 \text{ MPa} \) and \( C_t = 1 \)) our models predict \( 10^{-6} < \gamma_d < 10^{-5} \text{ J m}^{-2} \). For comparison, the energy per unit length of a dislocation in an elastically isotropic material is given by (e.g. Kohlstedt & Hansen 2015)

\[ \gamma_d = \frac{Gb^2}{4\pi(1 - v)} \frac{r}{r_c}, \]  \quad (100)

where \( r \) is the mean spacing between dislocations, approximated as \( r \approx 1/\sqrt{\omega} \), \( r_c \) is the radius of the dislocation core, typically set at \( r_c \approx b \), and the rest of the parameters defined in Table 1. Using values typical for olivine, as in Table 1, and equilibrium dislocation density range \( 10^6 \text{ m}^{-2} < \omega < 10^9 \text{ m}^{-2} \), as predicted by our model for \( \tau_d = 1 \text{ MPa} \) (Fig. 1), (100) yields \( \gamma_d \) on the order of \( 10^{-8} \text{ J m}^{-2} \), which implies \( \alpha \approx 10^{-5} < \alpha_{cr} \). Thus, material deforming at an applied stress of \( \tau_d = 1 \text{ MPa} \) would not develop sufficient density of intragranular defects to offset grain growth.

Doing the same calculation for \( \tau_d = 100 \text{ MPa} \), we get \( 10^{10} < \omega < 10^{13} \text{ m}^{-2} \) (Fig. 1) and \( \alpha_{cr} \approx 5 \times 10^{-6} \). The value of \( \gamma_d \) from (100) is still approximately \( 10^{-8} \text{ J m}^{-1} \) (as it scales only weakly with \( \omega \) according to (100)), which yields \( \alpha \approx 10^{-5} > \alpha_{cr} \). Thus, material deforming at an applied stress of \( \tau_d = 100 \text{ MPa} \) (or, according to Fig. 3, at \( \tau_d > 60 \text{ MPa} \)) can reach a finite steady-state grain size, which will be governed by the balance in energies associated with the grain boundaries and the intragranular defects.

6 DISCUSSION

6.1 Offsetting grain growth in Earth like rocks

Using the simple two-grain model in Section 3, we demonstrated that, depending on the value chosen for \( \alpha \), the grain growth can be unstable (the larger grain keeps on growing until the smaller grain is consumed) or stable (the two grains reach a steady-state size and dislocation density). Specifically, there exists a critical value for \( \alpha \) (\( \alpha = \alpha_{cr} \)), such that when \( \alpha > \alpha_{cr} \) the system can reach a stable equilibrium. In the more general model with many grains, albeit with the simplifying assumptions of homogeneous stress and a dislocation density that depends instantaneously on grain size, we demonstrated in Section 5 that, analogous to the two-grain model, the value of \( \alpha \) determines the fate of the grain size distribution.

6.2 Oscillating grain size: characteristic timescale and rheological inferences

While the simplifications of the many-grains model did not allow for a varying rates of dislocation density evolution, we could use the simple two-grain model in Section 3 to analyse the coupling of the timescales associated with dislocation kinetics and grain growth. We demonstrated that for certain values of \( \alpha \) (namely, \( \alpha > \alpha_{oe} \)), the system can oscillate as it converges towards its stable equilibrium state. The dimensional oscillation frequency is of the order of \( 1 - 10 \times 10^{-4} \text{ s}^{-1} \) (Fig. 4), which holds both for the shown \( \tau_d = 1 \text{ MPa} \), as well as for \( \tau_d = 100 \text{ MPa} \), but using \( \beta \) on the order of \( 10^{-2} \), which corresponds to about three full cycles per 1 to 10 yr.
When material deforms in grain size sensitive creep regime (e.g. diffusion creep), such oscillations will manifest themselves as rheological strengthening and weakening, as was also alluded to in Karato (1989). Experimental studies on hot deformation of metals, in particular nickel, also demonstrate transient fluctuations in material strength, between work-hardening when static recrystallization (i.e. diffusive grain growth) dominates and softening when dynamic recrystallization dominates (Sellars 1978), which eventually converges towards a steady state.

Our predicted timescale of 1 to tens of years for the oscillations in grain size, and thus potentially also material strength, can have implications for geological processes such as transient aseismic creep. A sudden stress load from an earthquake, which would lower the value of $\alpha_{\text{osc}}$ needed for the mineral grains to be in oscillatory
regime, can induce oscillations in material strength and deformation rate. It may take decades before the system, after undergoing a few oscillations, reaches its steady state. The effect of grain size on transient strain-weakening and -strengthening, and the resulting post-seismic creep of ductile shear zones following an episode of time-variant earthquake-like elastic load, has been demonstrated in (Montési & Hirth 2003). Including grain-size oscillation with its annual and decadal timescales in a post-transient creep model may reveal oscillatory behaviour during aseismic response.

A better constraint on the dislocation kinetics (i.e. the value of \( \beta \) in our model), for example, from experimental studies, would be useful to assess which processes, from rapid earthquakes to the relatively slow movement of tectonic plates, could potentially interact with the microphysically controlled timescales of grain growth and shrinkage.

### 6.3 Comparison to other grain damage models

The essential physics entering grain damage models (e.g. Bercovici & Ricard 2005; Austin & Evans 2007; Ricard & Bercovici 2009; Rozel et al. 2011) is that if no work is being done on the grains, then the grains will grow and the mean grain size will increase. Meanwhile, if deforming work is being pumped into the system, then some small fraction of that energy (the part that does not go to heat) will be converted to and stored as recoverable energy. In monomineralic polycrystalline rocks, the stored energy can take the form of increased grain boundary area (through dynamic recrystallization and formation of new smaller grains and subgrains) or increased density of intragranular defects, such as dislocations. The generation of dislocations is an intermediate step in forming the new recrystallized grains, as they group to form subgrains and eventually new grains (this is, of course, in addition to the free dislocations that reside in the grains’ interior). The stored energy residing in either dislocations or grain boundaries affects subsequent grain growth, as was also demonstrated in this study. The previously published grain damage models do not explicitly account for dislocation processes that lead to dynamic recrystallization, but rather assume that a fraction of deforming energy is immediately converted into new grain boundary energy. Our model explicitly accounts for the effect of dislocation dynamics on grain size evolution and thus aims to model this energy conversion more physically consistently. Just how much of the deforming work goes towards forming the new grains, a quantity known as the damage partitioning fraction, is one of the least well experimentally constrained physical properties entering the grain damage models (Rozel et al. 2011; Mulyukova & Bercovici 2017). The model presented in this paper facilitates the comparison between the predictions of the theoretical models (i.e. grain size and dislocation density) and experiment on dynamic recrystallization, and can thus potentially lead to a better constrained damage partitioning fraction. However, while our model addresses an important intermediate step in forming the new grains, it currently excludes the discontinuous process of grain splitting, which would have to be incorporated if we were to exactly compare our model to the previously published grain damage models.

### 7 CONCLUSIONS

We presented a model of grain size evolution, where the processes of grain growth and grain size reduction by dynamic recrystallization are governed by the competition between grain boundaries and intragranular defects (dislocations) to reduce the grains net internal energy. We demonstrated that the increase in the grain’s internal energy due to the presence of dislocations can act to stabilize grain growth, thus allowing for finite equilibrium grain sizes. Intragranular defects were shown to offset grain coarsening both in the simple two-grain model, where dislocation density could evolve in time, and with the many-grains model involving a grain size distribution, but where the dislocation density was only dependent on grain size and not on time. We concluded that for lithospheric rocks, the applied stress needs to be sufficiently high (e.g. \( \tau_d > 60 \text{ MPa} \)) for the energy associated with dislocations to offset grain growth.

We explored the effect of stress variation between the grains and the timescale of dislocation dynamics (in particular, the rate at which dislocation density reaches its steady state) with the simplified two-grain model. The results from the two-grain model infer that grains within the same material can be stable at different sizes if the stress is allowed to vary between them. Furthermore, the competition of two different timescales—that of diffusion-controlled grain growth and the dislocation kinetics—can lead to oscillating behaviour on timescales of 1–10 yr as the grain size and dislocation density advance towards their steady states. The effect of these oscillations on the rheology of lithospheric rocks, for example, their strengthening and weakening through time, as we all their potential application to geological processes such as post-seismic creep in ductile shear zones, is subject to future studies. The theoretical model needs further development in order to test these inferences for larger systems,
that is, for an ensemble of grains. Future models of grain size evolution should also include a distribution in dislocation density as independent of grain size, as well as the effect of discontinuous grain growth and damage (i.e. microcracking and coalescence of grains), and the contribution of mechanical work to grains entropy.

One of the implications from our model is that accounting for dislocation dynamics helps keep the grain size smaller than if the grain boundary energy was the only driving force for grain boundary migration. In a lithospheric setting, smaller grain size, or slower grain growth, means that it would require less mechanical work to establish weak localized shear zones through grain damage, and allow for a longer survival of those weak zones.

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REFERENCES


