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Influence of dihedral angle on the seismic velocities in partially molten rocks

Saswata Hier-Majumder *, Matthew E. Abbott

Department of Geology, University of Maryland, College Park, MD 20742, USA

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ABSTRACT

This article reports the influence of dihedral angle in a partially molten aggregate on its effective elastic properties using theoretical techniques. For a given mineral assemblage, dihedral angles can vary widely depending on the composition of the melt. Our results indicate that wetting melts with low dihedral angles have a lower fraction of intergranular contact area, contiguity, reducing the effective elastic moduli. An important consequence of this effect is that the seismic signature of an aggregate with a small volume fraction of a wetting melt will be similar to that of an aggregate containing a larger volume fraction of less wetting melt. Inferring the extent of melting in seismic ultralow velocity zones, therefore, needs to incorporate the influence of melt composition via the influence of dihedral angle.

1. Introduction

Earth's deep interior is characterized by a number of low seismic velocity zones. As they pass through these regions, both *S* and *P* wave velocities decline greatly, with *S* waves slowing down more than *P* waves. A number of thin patches of such ultralow velocity zones (ULVZ) have been observed at the Earth's core–mantle boundary (Hutko et al., 2009; Rost and Revenaugh, 2003; Rost et al., 2005; Williams and Garnero, 1996). Typically, the magnitude of the velocity reductions in the ULVZ is ascribed to the melt volume fraction or the degree of melting. A body of recent theoretical and experimental works demonstrates that the fractional area of intergranular contact, contiguity, of a partially molten aggregate exerts the primary control on their effective elastic properties (Hier-Majumder, 2008; Takei, 1998, 2000, 2002). While the melt volume fraction or the degree of melting controls the contiguity of a partially molten aggregate, other controls on the contiguity are also capable of influencing the seismic velocities.

Besides contiguity, another important textural quantity in partially molten rocks is the dihedral angle at grain–melt interfaces. The dihedral angles in a given mineral matrix are sensitive to the chemical composition of the melt. For example, under upper mantle conditions, basaltic melts subtend a dihedral angle of approximately 34° (Cooper and Kohlstedt, 1982) while an aqueous fluid subtends an angle of 76° (Hier-Majumder and Kohlstedt, 2006), in an olivine-rich matrix. A recent compilation of laboratory experiments on the steady-state microstructures indicate that the contiguity in partially molten rocks display a systematic variation with dihedral angles (Yoshino et al., 2005). Such a variation in contiguity and dihedral angle also influences the seismic velocities of these melt and fluid bearing rocks. Evidence from direct measurement of seismic velocity in partially molten analogue materials with controlled dihedral angles, also supports this inference (Takei, 2000). In aggregates with low dihedral angles, both shear and *P* waves travel slower than through aggregates containing the same melt fraction but a higher dihedral angle (Takei, 2000). These experimental results indicate that besides the degree of melting, variation in melt composition (through dihedral angle) can also produce a distinct seismic signature.

Following a recent work (Hier-Majumder, 2008), this article explores the correlation between the dihedral angle and contiguity in a partially molten aggregate. The model incorporates dynamic interaction among a number of contiguous grains surrounding a melt pocket in two dimensions. Interfacial tension along grain–grain and grain–melt interfaces excites a viscous flow in the interior of the grains and the melt pocket until a steady-state microstructure is reached (Hopper, 1990, 1993a,b; Kang, 2005; Kuiken, 1993).The viscous flow within the grains, part of a process named viscous sintering, is controlled by the conservation of mass and momentum within each grain and the melt pocket, supplemented by suitable boundary conditions. We employ a boundary integral formulation to solve the governing nonlinear equations in a hexagonal grain geometry. This numerical solution is also supplemented by an analytical solution for pressure, velocity, and steady-state grain shape in an aggregate with a four-fold packing symmetry. Contiguity and dihedral angles measured from the numerical experiments are compared with experimental measurements of contiguity by Yoshino et al. (2005).

* Corresponding author. Tel.: +1 301 405 6979.
E-mail address: saswata@umd.edu (S. Hier-Majumder).

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Finally, we calculate the elastic moduli and seismic velocities of the aggregates from the numerical models, and discuss the implications for Earth's deep interior. The results from our numerical models are also compared to the direct measurement of the influence of dihedral angle on seismic velocity by Takei (2000).

2. Methods

A detailed derivation of the formulation is presented in a previous article (Hier-Majumder, 2008). Only essential equations are outlined here. In this article, we present two sets of solutions. In one set of analysis, we present analytical solutions for the velocity, pressure, and steady-state shape of a grain immersed in the melt and acted upon by surface tension, representing a four-fold symmetry. In the second set, we present a two-dimensional numerical solution for the steady-state shape of a melt pocket surrounded by three grains. Governing equations for each case is described in Section 2.1. Sections 2.2 and 2.3 outline the new features of the numerical model and the method used to measure contiguity and dihedral angles from our numerical experiments.

2.1. Governing equations

Consider a collection of N viscous grains immersed in a viscous melt. The shape of the k-th grain is described by the function $F^k(\boldsymbol{r},t)=0$, where $\boldsymbol{r}$ is the position vector. Conservation of mass and momentum within each grain and the melt are given by

$$\nabla\cdot\boldsymbol{u}^i=0, \tag{1}$$

$$\nabla\cdot\mathbf{T}^i=0, \tag{2}$$

where $\mathbf{T}^i$ and $\boldsymbol{u}^i$ are the stress tensor and velocity vector within the k-th grain ($i=k$) or melt ($i=m$). The stress tensor is related to viscosity μ^i and pressure P^i by the linear constitutive relation,

$$\mathbf{T}^i=-P^i\mathbf{I}+\mu^i\left(\nabla\boldsymbol{u}^i+\left(\nabla\boldsymbol{u}^i\right)^T\right), \tag{3}$$

where $\mathbf{I}$ is the identity matrix.

The governing equations are solved with a no-slip boundary condition on the interface, Γ^k, of the k-th grain, (Kim and Karilla, 2005; Leal, 1992; Pozrikidis, 2001)

$$\boldsymbol{u}^k=\boldsymbol{u}^m. \tag{4}$$

In addition, traction across the grain interface is supported by the force balance boundary condition (Leal, 1992, Ch. 5),

$$\Delta\mathbf{T}^k\cdot\hat{\boldsymbol{n}}^k+\left(\mathbf{I}-\hat{\boldsymbol{n}}^k\hat{\boldsymbol{n}}^k\right)\cdot\nabla\gamma-\gamma\hat{\boldsymbol{n}}^k\left(\nabla\cdot\hat{\boldsymbol{n}}^k\right)=0, \tag{5}$$

where $\Delta\mathbf{T}^k$ is the difference in stress across the surface of the k-th grain, $\gamma(r)$ is the interfacial tension, and $\hat{\boldsymbol{n}}^k$ is the unit normal vector. The first term in Eq. (5) arises from the difference in traction across the interface, the second term arises due to variation of surface tension along the interface, and the last term arises from curvature driven surface tension force, where the principle curvature of the interface is given by $\nabla\cdot\hat{\boldsymbol{n}}^k$ (Kim and Karilla, 2005; Leal, 1992; Pozrikidis, 2001). The tensor $\left(\mathbf{I}-\hat{\boldsymbol{n}}^k\hat{\boldsymbol{n}}^k\right)$ extracts the surface parallel component of the gradient in surface tension. The normal component of the vector Eq. (5) consists of the first and the last terms, indicating that the normal traction is balanced by curvature and the surface tension. This condition is also known as the Laplace condition. The tangential component of the boundary condition consists of the first two terms, indicating variation of tension along the surface is balanced by a drop in the shear stress across the boundary. This is known as the Marangoni effect (Leal, 1992).

Finally, the change in the shape of the k-th grain with time is constrained by the kinematic condition,

$$\frac{\partial F^k}{\partial t}+\boldsymbol{u}^k\cdot\nabla F^k=0. \tag{6}$$

In the steady-state, textural equilibrium is attained and the first term on the left hand side of Eq. (6) becomes zero.

The surface unit normal $\hat{\boldsymbol{n}}^k$ depends on the unknown shape function F^k of the k-th particle. Consequently, Eq. (5) is strongly nonlinear. In the following two sections we present a linearized equation governing the shape of each grain and a numerical technique for solving the nonlinear equations by converting the differential equations into a boundary integral equation.

2.1.1. Analytical solution

Consider a grain, immersed in the melt. In the first order, influence of the surrounding grains on this grain is manifested by an alteration of the surface tension at the intergranular contact (Hier-Majumder, 2008). Variation of the surface tension along the interface of the grain leads to a drop in shear stress and drives Marangoni flow, until the steady-state is reached. For simplicity, we assume that the unperturbed shape of an isolated grain immersed in melt is spherical. In the limit of small deformation, a small perturbation of the spherical shape takes place.

In the spherical polar coordinate system, assuming axial symmetry, the shape distortion takes place only along the colatitude, θ. Thus, the shape of the grain is given by

$$F(\boldsymbol{r})=r-a-\epsilon f(\theta), \tag{7}$$

where $f(\theta)$ is an unknown shape function, a is the radius of the initial sphere, and $\epsilon\ll1$, is a constant. The unit normal at a point on the surface of this perturbed shape is,

$$\hat{\boldsymbol{n}}=\frac{\nabla F(\boldsymbol{r})}{|\nabla F(\boldsymbol{r})|}=\hat{\boldsymbol{r}}-\epsilon\nabla f(\theta), \tag{8}$$

where $\hat{\boldsymbol{r}}$ is the unit radial vector. The deviation from the unperturbed state is caused by introducing a small perturbation $\gamma_1(\theta)$ to the surface tension,

$$\gamma=\gamma_0+\epsilon\gamma_1(\theta), \tag{9}$$

where γ_0 is the interfacial tension in the unperturbed state. Since γ_0 is constant, the velocities within the grain and the melt are zero in the unperturbed state, rendering the zeroth order stress jump condition in Eq. (5) as

$$\Delta P_0=\frac{2\gamma_0}{a}. \tag{10}$$

The analytical solution to the perturbed pressures, velocities, and the shape function in Eqs. (1), (2), and (6), are obtained by using Lamb's solutions techniques (Lamb, 1895), outlined in Appendix B. In brief, the pressures and velocities within the grain and in the melt are expanded in a series of harmonic functions with four unknown coefficients. The coefficients are determined from four boundary conditions: (1) continuity of tangential velocity at the grain–melt interface, zero normal velocity of the (2) grain and (3) the melt at the grain–melt interface, and (4) the tangential component of the force balance boundary condition (5). The solutions thus obtained, provide information regarding the velocity and the pressure fields, but the perturbed shape function $f(\theta)$ still remains to be solved.

We prescribe the perturbed surface tension $\gamma_1(\theta)$ as a sum of Legendre polynomials and expand the shape function $f(\theta)$ in a series of unknown functions. Substituting the pressure and velocity obtained