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ScienceDirect
Earth and Planetary Science Letters 267 (2008) 32–44
EPSL
www.elsevier.com/locate/epsl

Numerical models of stiffness and yield stress growth in crystal-melt suspensions

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Received 21 June 2007; received in revised form 31 October 2007; accepted 13 November 2007
Available online 3 December 2007
Editor: C.P. Jaupart

Abstract

Magmas and other suspensions that develop sample-spanning crystal networks undergo a change in rheology from Newtonian to Bingham flow due to the onset of a finite yield stress in the crystal network. Although percolation theory provides a prediction of the crystal volume fraction at which this transition occurs, the manner in which yield stress grows with increasing crystal number densities is less-well understood. This paper discusses a simple numerical approach that models yield stress in magmatic crystalline assemblies. In this approach, the crystal network is represented by an assembly of soft-core interpenetrating cuboid (rectangular prism) particles, whose mechanical properties are simulated in a network model. The model is used to investigate the influence of particle shape and alignment anisotropy on the yield stress of crystal networks with particle volume fractions above the percolation threshold. In keeping with previous studies, the simulation predicts a local minimum in the onset of yield stress for assemblies of cubic particles, compared to those with more anisotropic shapes. The new model also predicts the growth of yield stress above (and close to) the percolation threshold. The predictions of the model are compared with results obtained from a critical path analysis. Good agreement is found between a characteristic stiffness obtained from critical path analysis, the growth in assembly stiffness predicted by the model (both of which have approximately cubic power-law exponents) and, to a lesser extent, the growth in yield stress (with a power-law exponent of 3.5). The effect of preferred particle alignment on yield stress is also investigated and found to obey similar power-law behavior.

PACS: 91.40.Hw; 91.40.La; 91.55.Ax
Keywords: gneiss domes; magma rheology; continuum percolation; yield stress; suspension; partial melt

1. Introduction

Magmas and other crystal-melt suspensions are complex multiphase materials that often contain networks of solid crystal particles (e.g., Marsh, 1981; Cashman and Blundy, 2000). The particles in magma complicate its rheology — affecting viscosity, and adding porous medium flow conditions around crystal networks to bulk material flow conditions (Kerr and Lister, 1991; Stein and Spera, 1992; Lejeune and Richet, 1995). Magmas with sufficiently high particle concentrations exhibit shear thickening (Smith, 2000), and eventually the onset of yield stress (Saar et al., 2001). At yet higher concentrations, yield stress increases as particles are added until a completely solidified rock exists (Petford, 2003). Understanding the complexities of magma rheology that arise from magma composition is key to understanding a range of magmatic processes, such as partial melt migration and melt expulsion from, or movement with, the solid matrix. These processes can occur in gneiss domes, mantle plumes, and partial melts below mid-ocean ridges or within mantle wedges (e.g., Hirth and Kohlstedt, 1996; Kelemen et al., 1997; Teyssier and Whitney, 2002; Whitney et al., 2003). Further examples include: melt

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0012-821X/$ - see front matter
doi:10.1016/j.epsl.2007.11.028

expulsion in plutons; lava lake solidification; volcanic magma and surface lava flow emplacement; volcanic conduit plug formation; magma fragmentation; and magmatic volatile degassing (e.g., Marsh, 1982; Gardner et al., 2000; Paterson, 2001; Thompson et al., 2001; Jellinek and Kerr, 2001; Blundy et al., 2002; Rust et al., 2003; Bachmann and Bergantz, 2004; Blundy and Cashman, 2005; Marsh, 2006; Hammer, 2006; Gonnermann and Manga, 2007).

At low number densities, the effects of particles on magma viscosity are described by the Roscoe–Einstein relations (Einstein, 1906; Roscoe, 1953). At higher densities, crystals link to form a macroscopic sample-spanning crystal network or percolating backbone (Philpotts et al., 1998), resulting in the onset of yield stress in the material (Kerr and Lister, 1991; Saar et al., 2001; Jerram et al., 2003). This transition from Newtonian to Bingham fluid can be predicted via percolation-theoretic approaches (Stauffer and Aharony, 1992; Saar and Manga, 2002). However, the role of crystals in developing increased magmatic yield stress for crystal volume fractions that exceed the percolation threshold is less-well understood, particularly when intergrowing and non-spherical particles are considered.

Onset of yield stress in magmas has been estimated to occur at volume fractions anywhere between 15% and 50%; estimates of the value of the yield stress in this range vary by several orders of magnitude (Kerr and Lister, 1991; Petford and Koender, 1998; Hoover et al., 2001; Petford, 2003). This is in part due to the difficulties of measuring yield stress (Nguyen and Boger, 1992; Moller et al., 2006), and partially due to variations between samples. Partial melt experiments by Hoover et al. (2001) demonstrate that magmas with more anisotropic-shaped particles develop yield stress at smaller volume fractions than those with more equant particles. The rheology of magmas with high crystal number densities may also be influenced by particle orientation (Bagdassarov and Pinkerton, 2004; James et al., 2004). Studies of colloidal systems demonstrate that particle alignment is a contributing factor to the rheology of suspensions of prolate (Shaqfeh and Fredrickson, 1990) and oblate (Jogun and Zukoski, 1999) particles. Yield stress is also affected by the presence of bubbles in the melt, which contribute to magma rheology both directly through interactions between bubbles (Ryerson et al., 1988; Gardiner et al., 1998) and indirectly by rearranging the crystal network (Walsh and Saar, in preparation).

It can be difficult to control and isolate effects from the many sources that contribute to magma rheology, and it is often impossible to obtain data on transient crystal-scale behavior in real materials. Accurate numerical simulations enable investigation of the rheology of these materials without being subject to a number of the difficulties encountered in experimental approaches. Numerical simulations allow a variety of different particle shapes and orientations to be investigated, and crystal-scale data to be gathered with relative ease. Although simulated results will never replace real-world data, numerical models offer an important adjunct to experiments that allow greater insight into the underlying physical processes.

This paper presents a simple numerical model that aims to reproduce the development of yield stress in bonded crystal assemblies. In this model, crystals are represented by soft-core interpenetrating cuboid (rectangular prism) particles, as outlined in Section 2. These assumptions were previously adopted by Saar et al. (2001) to investigate the transition from Newtonian to Bingham flow in magmas. In this paper, the subsequent increase in yield stress due to increasing particle volume fractions is simulated using a network model given in Section 3. This model accounts for interparticle bond strength and fracture with a network of interparticle springs, providing estimates of assembly stiffness and yield stress, respectively. Here, we assume i) that the interparticle-spring stiffnesses are proportional to the overlap of the cuboid particles; ii) that the particle bonds have a high level of rotational resistance, allowing them to resist buckling motion; and iii) that the bonds fail if the contacting particles' relative motion exceeds a preset limit. This approach does not account for the contribution to the yield stress from the interparticle fluid. In Section 4, this approach is used to investigate the influence of different factors on the yield stress of crystal networks with particle densities above the percolation threshold. In particular, we examine the relationship between the yield stress and growth in the average number of bonds per particle, the mean bond strength of the percolating backbone based on particle overlap, and the material stiffness. The effects of particle shape and orientation on yield stress are investigated, and the results of the model compared with estimates obtained from critical path analysis. Conclusions are discussed in Section 5.

2. Soft-core crystal network

In the current model, the crystal network is represented by an assembly of equal-sized cuboid particles, whose orientations are chosen randomly from a predetermined distribution, Φ. Overlapping crystals are allowed to interpenetrate fully, resulting in a soft-core model of crystal contact that simulates crystal intergrowth in a zero-shear environment (Fig. 1). The spatial arrangement of particle centers is described by a Poisson distribution, such that the probability of finding k particles within a given volume, V, is

$$P(N(V)=k)=(nV)^k \exp(-nV)/k!, \tag{1}$$

where $N(V)$ is the number of particles within the volume and n is the particle number density. From Eq. (1), the average number of particle centers that lie within a region of volume V is $\sum_k kP(N(V)=k)=nV$, while the volume fraction, ϕ, of the overlapping particles is

$$\begin{aligned}\phi &= \sum_{k=0}^{\infty}\left(1-(1-v/V)^k\right)P(N(V)=k)\\ &= 1-\exp(-nv),\end{aligned} \tag{2}$$

where v is the volume of a single particle (Garboczi et al., 1991).

Soft-core particle systems are often employed in continuum percolation studies (Meester, 1996). Percolation theory describes the relationship between assembly interconnectivity and the shape, number density, spatial distribution, and orientation of the assembly's constituent objects. The geometric