A modeling approach to understanding the role of microstructure development on crystal-size distributions and on recovering crystal-size distributions from thin slices

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ABSTRACT

Computer modeling of microstructure development was used to determine whether competition for space among growing crystals modifies the crystal-size distribution (CSD) predicted by the crystallization kinetics. Microstructures were modeled with prisms, plates, and cuboids, respectively. In all cases, the true CSDs calculated from crystal volumes in the microstructure corresponded closely with the linear ideal CSDs predicted by crystallization equations indicating that grain impingements did not significantly modify the predicted CSD information. Crystal intersection widths and lengths were measured in 2-dimensional slices through the microstructures to test if the CSD information could be recovered. For prisms and plates, the recovered CSDs compared favorably with the true CSDs, but cuboids yielded mixed results depending on their shapes and need further study. For prisms, the recovered CSDs were linear and for plates slightly curvilinear. These results indicate that rocks with recovered, curvilinear CSDs should be interpreted cautiously as indicators of complex crystallization histories, and that petrographic examination should have precedence in such interpretations.

Keyword: Crystal-size distribution, CSD, microstructure, computer modeling

INTRODUCTION

Crystal-size distribution (CSD) theory was developed by Randolf and Larson (1971) to quantify industrial crystallization processes. The theory was adapted to magma crystallization by Marsh (1988, 1998) and Cashman and Marsh (1988), and others have since used it to reconstruct kinetic and dynamic models of magma emplacement and crystallization (Armienti et al. 1994; Higgins 1998; Zieg and Marsh 2002; Mock et al. 2003; Binde- man 2003). Although the theory is now generally accepted, Pan (2001) argued that CSDs contain a bogus pattern unrelated to the crystallization kinetics [see responses by Schaeben et al. (2002) and Marsh (2002)]. Nevertheless, the need for validation of CSDs recovered from microstructures is critical to advance and draw reliable conclusions. A few studies have dealt with this need (Castro et al. 2003; Binde man 2003; Gualda 2006; Mock and Jerram 2005). The present investigation addresses this need by comparing CSDs recovered from crystal intersection widths and lengths obtained in slices through microstructures with the true or actual CSDs calculated from the known crystal volumes.

Some of the early computer models simulated recrystallization in metals and ceramics graphically using small discrete area units (Anderson et al. 1986; Grest et al. 1986; Nasello and Ceppi 1986; Ohser and Muecklich 2000). More recent models have dealt with crystallization of igneous textures in both two and three dimensions. Elliott et al. (1997) measured dihedral angles between grains in slices to distinguish non-equilibrated textures, and Cheadle et al. (2004) measured porosity and permeability along grain boundaries to estimate the amount of trapped melt. Hershum and Marsh (2002) developed a 2-dimensional model using discrete area units to represent melt and solids and then compared textures formed by constant crystal growth and dispersive growth. Hershum and Marsh (2006) developed a 3-dimensional model in which Avrami crystallization controlled the timing of crystal nucleation and growth. Although their approach is fundamentally sound for continuous nucleation and growth processes, Avrami control appears to result in some timing problems between nucleation and growth when they are modeled in discrete time stages. Amenta (2001) and Amenta et al. (1992, 1997a, 1997b, 2002) developed 2- and 3-dimentional models in which crystals grew using their own internal lattice patterns as distinct from the voxel method of representing portions of crystals. The latter model, with recent modifications that incorporate crystal nucleation and growth laws, was used in the present investigation.

Crystal sizes measured from slices must be corrected for the intersection probability effect and the cut-section effect (Under- wood 1970). Corrections for the former are simple for spheres (Royet 1991), and correction schemes have been developed for other shapes (Saltikov 1967; Royet 1991; Peterson 1996; Sahagian and Proussevitch 1998). Corrections schemes for the latter are complex and highly dependent on crystal shapes (Saltikov 1967; Sahagian and Proussevitch 1998; Higgins 1994, 2000). Both corrections are incorporated in the program CSDCorrections (Higgins 2000), which was tested on tetragonal prisms and plates but apparently not on cuboids (rectangular parallelepipeds that have three unequal axes). The primary recovery method used in the present investigation is CSDCorrections and the secondary method for comparison is that of Underwood (1970) and Marsh (1988) that corrects only for the intersection probability effect.

Several studies have tried to identify the measurable param-