

# Modeling of crystal size distributions (CSDs) in sills

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## Abstract

A new model for the generation of crystal size distributions (CSDs) in igneous rocks is presented here. Synthetic or numerically simulated CSDs are generated with a growth rate that is proportional to the amount of precipitating solids and inversely related to the second moment of the CSD (total surface area) and with the  $\log(\text{nucleation rate}, I)$  vs.  $\log(\text{cooling rate})$  relationship of Cashman [Cashman, K.V., (1993). Relationship between plagioclase crystallization and cooling rate in basaltic melts. *Contrib. Mineral. Petrol.*, v. 113, pp. 126–142.] for crystal nucleation. The resultant CSDs resemble those observed in natural rocks. In the new model, growth rate is constrained by a mass balance and crystal population systematics; it is not calculated as a function of cooling rate or undercooling. The development of the numerical model was motivated in part by the failure of analytical modeling of crystal populations based solely on cooling rate to generate CSDs similar to those observed naturally. The new model is used to create a suite of CSDs from various positions within a sill; cooling and solidification of the sill are calculated numerically. The model reproduces many features observed in the CSDs of natural rocks such as linear CSDs in plots of  $\ln(\text{population density})$  vs. crystal size, ‘D’-shaped mean crystal size profiles and decreasing CSD intercept and slope magnitude (i.e.,  $|\text{slope}|$ ) with distance from the sill/wallrock contact, and the CSD intercept vs. slope relationship. The model suggests the use of inversion to more accurately determine residence time from a natural CSD.

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## 1. Introduction

Crystal size distributions (CSDs) are quantitative representations of crystal populations in rocks (Marsh, 1988; Cashman and Marsh, 1988; Mangan, 1990; Resmini and Marsh, 1995; Marsh, 1998) and provide information on the kinetics of crystal nucleation and growth in magmas and lavas. Natural CSDs are characterized to first-order as linear or quasi-linear

spectra with negative slope on a plot of the natural logarithm of population density vs. crystal size. Fig. 1 shows a CSD of plagioclase in a high-alumina basalt from Atka Island, Alaska (sample AT-67 of Myers et al., 1986, and of Resmini, 1993; Resmini and Marsh, 1993); additional examples of CSDs can be found in, e.g., Zieg and Marsh (2002), Zieg (2001), Marsh (1998), Cashman and Marsh (1988), Higgins (1996), Mangan (1990), and Resmini and Marsh (1995). Since crystal nucleation and growth are also responses to the cooling of molten rock, CSDs may also record the history of cooling of magmatic systems. It is difficult, however, to extract such information from CSDs because of a relative paucity of modeling studies which attempt to relate

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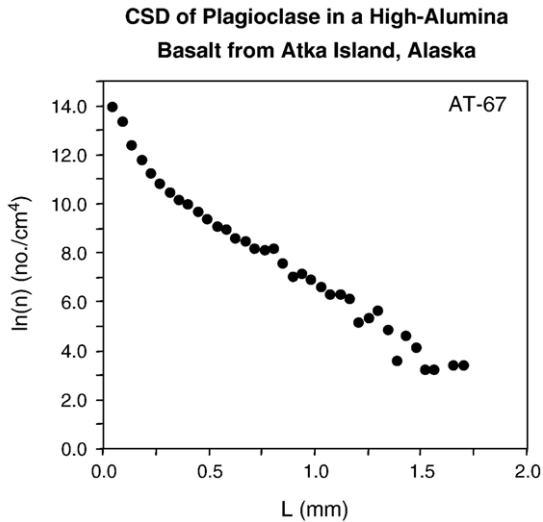


Fig. 1. A CSD of plagioclase in a high-alumina basalt from Atka Island, Alaska, from Resmini (1993).

CSDs to magmatic processes such as solidification and which can guide our understanding of natural systems (notable exceptions include Spohn et al., 1988; Hort and Spohn, 1991; Marsh, 1998). Alternatively, natural CSDs provide irrefutable criteria against which models of crystal nucleation and growth in magmatic systems must be checked. Here, a new model for the generation of CSDs is presented. It was motivated in part by testing the ability of a model of crystal nucleation and growth kinetics based on cooling rate to produce CSDs typical of those observed in rocks. It was also developed to implement a more complicated crystallization mechanism than one based on cooling rate alone.

Cashman (1993), following an extensive review of the literature on crystal nucleation and growth, has proposed that the logarithm of both the crystal growth rate,  $G$ , and the crystal nucleation rate,  $I$ , in magmatic systems such as sills, dikes, and lava lakes are functions of the logarithm of the cooling rate,  $\partial T/\partial t$ . Below, an analytical expression for the CSD in a system closed to mass transfer (e.g., a sill) is obtained as the solution to the batch population balance equation combined with a cooling and solidification model from Jaeger (1957) and the cooling rate-based logarithmic kinetic expressions. The resulting CSD does not resemble those typically observed in rocks.

In an attempt to understand the nature of the CSDs produced with the cooling rate-based (and other) kinetic expressions, a new model of CSD generation was developed. The new CSD model calculates a growth rate that is proportional to the amount of crystallizing solids and inversely dependent upon the evolving crystal

population, and employs the  $\log(I)$  vs.  $\log(\partial T/\partial t)$  relationship for crystal nucleation. The model is coupled to a model of cooling and solidification (with latent heat); the crystal growth rate is constrained by a mass balance and crystal population systematics. The resulting CSDs resemble those in natural rocks. This model is discussed in detail and is then used to create a suite of CSDs from various positions within a sill. The model reproduces many features observed in the CSDs of natural rocks such as linear CSDs in  $\ln(n)$  vs.  $L$  space, decreasing CSD intercept and slope magnitude (i.e.,  $|\text{slope}|$ ) with distance from the sill/wallrock contact, and the CSD intercept vs. slope relationship.

We begin by briefly describing the analytical calculations followed by a description of the numerical model. Implications of the new model for petrological analysis are then considered.

## 2. Analytical modeling: crystallization as a function of cooling rate

The batch population balance equation (BPBE) is a homogeneous, first-order, one-dimensional wave equation:

$$\frac{\partial n}{\partial t} + G \frac{\partial n}{\partial L} = 0 \quad (1)$$

which relates  $n$ , crystal population density (number/length<sup>4</sup>) to time,  $t$ , crystal growth rate,  $G$ , and crystal size,  $L$ . The BPBE lacks a term for the inflow and outflow of mass and is thus appropriate for modeling particulate processes such as crystal nucleation and growth in systems closed to mass transfer (Marsh, 1988; Randolph and Larson, 1988). When  $G$  is a function of  $n$ , Eq. (1) is quasi-linear. Solutions to Eq. (1) are thus of the form  $n=n(L,t)$ . Here, the method of characteristics (see, e.g., Lamb, 1995; Haberman, 1987) is used to analytically solve the BPBE (Eq. (1)) posed as a quasi-linear boundary value problem (i.e.,  $n(L,0)=0$  and  $n(0,t)=n^o(t)$ ). Derivation of the boundary conditions and growth rate term are described next.

### 2.1. BPBE boundary conditions and the crystal growth rate

Cashman (1993) has proposed the following kinetic expressions for describing the dependence of crystal nucleation and growth rates on cooling rate,  $\partial T/\partial t$ :  $\log(G)=\log(G') + p(\log(\partial T/\partial t))$  and  $\log(I)=\log(I') + m(\log(\partial T/\partial t))$ . The first expression, recast as  $G=G'(\partial T/\partial t)^p$ , provides the growth rate term for the BPBE and is also required for defining the boundary

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