Plagioclase population dynamics and zoning in response to changes in temperature and pressure

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Supplementary Material 1.

SNGPlag model equations for reducing temporary population of 120 crystal classes to a single class.

$$V_i = \sum_{\tau=1}^{120} N_\tau \, L_{a\tau} L_{b\tau} L_{c\tau}$$

Eq. 1

describes the total volume V_i of crystals nucleated over the 120 time steps τ composing the 12-hour time interval i-1 to i is the sum of the numbers N_τ and volumes (product of axis lengths $L_{x\tau}$) of crystals nucleated at each timestep τ.

$$N_i = \sum_{\tau=1}^{120} N_\tau$$

Eq. 2

gives the total number of crystals N_i nucleated in the interval i-1 to i.

$$v_i = V_i / N_i$$

Eq. 3

is the characteristic individual crystal volume.

$$V_\tau = N_\tau L_{a\tau} L_{b\tau} L_{c\tau} / V_i$$

Eq. 4

gives the fraction of new crystal volume (V_τ) that nucleated during each time step.

$$R_{aci} = \sum_{\tau=1}^{120} V_\tau L_{a\tau} / L_{c\tau}$$

$$R_{bci} = \sum_{\tau=1}^{120} V_\tau L_{b\tau} / L_{c\tau}$$

Eq. 5

provides characteristic ratios of a- to c- and b- to c-axis lengths for crystals nucleated during the interval i-1 to i.

$$L_{ci} = \left(\frac{v_i}{R_{aci} R_{bci}} \right)^{1/3}$$

Eq. 6

$$L_{ai} = L_{ci} R_{aci}$$

$$L_{bi} = L_{ci} R_{bci}$$

Eq. 7

give the characteristic c-, a-, and b-axis lengths for all crystals nucleated during i-1 to i. The characteristic surface area of the crystals can be easily calculated as the product of the a-, b-, and c-axis lengths. Equations 1-7 can be used to calculate characteristic crystal parameters of the total crystal population at any time by summing over the interval 1 to i for all crystals.

Supplementary Material 2.

File type: pdf

Sensitivity testing of SNGPlag model results to variation in nucleation, growth, and dissolution rates for a ~560 year time series with recharge events every 50 years. A) Temperature, B) pressure, and C) equilibrium anorthite composition time series for the model runs. D) and E) C-axis core-to-rim lengths through time. Both growth and nucleation rates exert strong controls on crystal size, with elevated nucleation rates resulting in decreased crystal sizes through time. In this example, even the nominal rates (N1G1D1) result in decreasing crystal size through time. F) and G) Core-to-rim c-axis compositional transects only show repeated zones of increasing and decreasing An content for scenarios that show increased crystal size through time (scenarios with suppressed nucleation rate). H) fractional cumulative crystal thickness as function of anorthite content. The peak at An68 for most crystals is an artifact of initializing the model runs with An68 antecrysts. I) Comparison of the input conditions (magenta) and those recorded by the final crystals. J) Ratio of recorded to input times as a function of anorthite content. K), L), and M) Total fraction time recorded versus growth, nucleation, and dissolution rates. Lines used in panels D-J are defined in panels D and E; symbols used in panels K-M are given below panel M. Run conditions are abbreviated as, for example, N10G10D01 to show nucleation and growth rates multiplied by 10 and dissolution rate multiplied by 0.1 (01 in the symbols indicates 0.1 and 004 indicates 0.004).

Supplementary Material 3.

File type: pdf

Explanation of shape plots displayed in Figures 5, 6, and 9. A) Crystal shapes are defined by the L_a/L_c and L_b/L_c ratios of crystal lengths, such that the shape of any crystal can be plotted as a vertical line with a maximum value of L_b/L_c, and minimum of L_a/L_c. The values for each crystal are shown as the vertical black lines, and the ratios L_a/L_c and L_b/L_c are shown as the dotted lines bounding the gray region. Example crystals are shown for a broad range of shapes, from acicular or elongate crystals with low values of both L_a/L_c and L_b/L_c, through tabular crystals with a broad range between the two ratios, to equant crystals with both ratios near 1. B) Characteristic a-, b-, and c-axis lengths of crystals from the cyclic heating run with increasing temperature magnitude shown in Figure 9. C) Shape plot from Figure 9 with the characteristic crystal shapes shown schematically over the course of the simulation.

Supplementary Material 4.

File type: mp4

Animation of 5269-year crystallization history. The crystal shown here has voxel sizes of 0.2 μm, and has been sectioned 2, 3, and 6 μm off center with respect to the a-, b-, and c-axes. The section has been rotated 30, 75, and 45 degrees about the a-, b-, and c-axes, respectively. In the animation, the long crystal axis is 15 degrees from parallel to the c-axis, and the short crystal axis is half-way between the a- and b-axes. The crystal is animated at a rate of 1 frame per year. The gray scale values in the left panel correspond to An content (brighter values are more anorthitic); the advancing gray bar near the bottom of the panel shows progress through the time series. The temperature time series is shown in the upper panel, with progress indicates in red.

The lower right panel shows the compositional profile (An content) as measured from core to rim following the yellow line shown on the left panel.

Supplementary Material 5.

File type: pdf

A) Temperature time series for a 5220-year interval with 273 total recharge events and 16 eruptions or decompression events occurring in 26 episodes. B) C-axis crystal length for V_{input}=0-0.5 (black line) and V_{input}=0-0.2 (blue line). Although the series with higher V_{input} does decrease to a length of 0 at ~1200 years, crystal growth outpaces dissolution through the remainder of the history. The low V_{input} series, however, never achieves lengths >20 μm, but repeatedly grows and dissolves the same portion of crystal.