Summary

Magmatic processes are major agents responsible for the formation and differentiation of the Earth's crust. In contrast to extensive efforts to improve understanding and utility of igneous geochemistry, physical processes of magma differentiation and solidification remain largely unclear. Large variability of igneous textures provides record of these processes and intensive parameters governing the crystallization. In this thesis, we develop quantitative methods, which allow us to better interpret igneous textures in the framework of physics of solidification.

We have developed a new three-dimensional model of crystallization from one-component melt driven by homogeneous and heterogeneous nucleation and crystal growth. The predicted textures are quantitatively characterized by crystal size distributions, spatial distribution functions and parameters representing grain contact relationships. The model employs high resolution in a large volume simulation domain in order to produce statistically stable results.

Our simulations, performed for various functional forms of nucleation and growth rates with respect to time, imply that (*i*) crystals are ordered (anti-clustered) on short length scales. This reflects that other crystals already have a finite size at the time of nucleation of younger crystal, and nucleation is hence suppressed on some length scale, since it only takes place in melt; (*ii*) cross sections with large apparent axial ratio, that is, elongate grain sections, are exponentially uncommon than equant shapes. Also, more elongate sections are frequently found for smaller hence interstitial crystals. Exact shape of the distribution of axial ratios is not very sensitive to nucleation and growth rate curves; (*iii*) log-linear crystal size distribution (CSD) curves are produced by a wide range of nucleation and growth rate functions; the most simple example being the constant growth rate and the exponential nucleation rate; (*iv*) bell-shaped Gaussian rates can produce nearly log-linear CSDs only if the growth rate reaches its maximum before the nucleation rate does. Increasing displacement of maxima of both rates promote the log-linear nature of the resulting CSD, and it finally predicts a hemicrystalline texture with residual melt, if the growth rate declines to zero before the nucleation rate reaches high enough value. From Gaussian rates, only these with high misfit, and hence with tendency to hemicrystallinity, lead to realistic textures. Therefore we propose that Gaussian

rates can only be a viable first-order model of the crystallization history for rapidly cooled magmas, where it represents increase of both rates due to increasing undercooling below the liquidus followed by kinetic suppression of both rates due to temperature decrease; (*v*) there exist two scalar parameters identified from grain contact relationships, that are independent of the crystallization history. These are slope and intercept of an average neighbor distance and neighbor number dependence on crystal size, respectively. In future applications, such parameters may aid in recognizing the magnitude of heterogeneous nucleation or the intensity of mechanical redistribution of crystals in natural settings; (*vi*) different combinations of the nucleation and growth rate curves may lead to textures with identical CSDs. Based on our numerical findings we expect, that such textures have also other parameters comparable. Therefore a CSD provides full characterization of a texture formed by homogeneous nucleation and growth of crystals. Due to this we conclude that a CSD is a function from which the both rates of nucleation and growth cannot be recovered simultaneously.

Time dependence of the nucleation and growth rates can be derived from CSD, if additional constraints such crystallinity-time function are used. We derive numerical apparatus to obtain a unique solution for both the rate of growth and nucleation when such constraints are imposed. Our calculations for quasi-linear crystallinity-time functions suggest that (*i*) the rate of nucleation is an increasing function with time; (*ii*) the growth rate reaches very high values at very low and high crystallinities, respectively. In these limits, the area of solid-liquid interface is small and hence high growth rate are expected in order to produce a finite increment of crystallinity; (*iii*) at moderate crystallinities, when the area of the solid-liquid interface is the largest, the growth rate decreases to low values and the system is expected to be close to thermodynamic equilibrium.

Calculated near-equilibrium growth rate can be converted into real units, if relevant cooling model is employed and the total crystallization span is bracketed by liquidus and solidus temperatures, respectively. For cooling of a deep seated, infinite sheet (dyke) of magma, the growth rate scales inversely with magma body thickness, and it increases non-linearly from the center to the margin of the body. The growth rate also depends on the CSD slope, whereby the steeper CSD slope results from a lower growth rate if other parameters are kept constant. Scaling to conditions relevant to those of Hawaiian lava lakes yields growth rates in order of 10^{-11} cm s^{-1}, which is in a good agreement with natural observations. The growth rate can be converted to growth time for any grain size of interest. In log-linear CSDs, growth time of the volumetrically most abundant grain size varies from 1/10 of characteristic cooling time for crystals in the pluton interior to 1/400 for those near the margin. Relative growth time thus depends on the location of the grain only and it is related neither to the CSD slope nor to the magma body size. From the growth rate and growth time, crystal travel

distance in a viscous magma due to action of gravitational force can be estimated. The crystal travel distance increases quadratically with the magma chamber size, thus revealing crystal settling is most efficient in large reservoirs. For kilometer-sized magma bodies, we predict that crystals can move across half of a magma chamber during their growth time even when magma viscosities are as high as 10^9 Pa s.

We apply quantitative textural analysis to the Smrčiny/Fichtelgebirge granite batholith (Czech Republic/Bavaria) in order to interpret its crystallization history. Six samples from distinct intrusive units and textural varieties were compared to simulated textures. The results indicate significant role of clustering of crystals in all samples as evidenced by spatial distribution functions and grain contact characteristics. The intensity of clustering is highest for like phase pairs but it remains lower for unlike pairs. We suggest that crystal clustering could have been produced by heterogeneous nucleation or by mechanical aggregation of crystals during crystal settling. The origin of clusters by mechanical aggregation of grains is supported by relatively lower degree of clustering observed in a sample representing rapidly crystallizing roof facies of the porphyritic Weißenstadt-Marktleuthen granite. The CSD curves for quartz, plagioclase, K-feldspar, muscovite, and biotite reveal concave-up nature of most CSDs, with the exception of the roof facies of the porphyritic Weißenstadt-Marktleuthen granite, which is characterized by straight CSD curves implying simple crystallization history. In some concave-up CSDs, two straighter segments are distinguish, which correspond to coarser and finer crystal populations, respectively. The bent CSDs are usually interpreted as a result of mechanical mixing of multiple crystal populations. In our case, however, the coarser grained population constitutes approximately 90 % of the magma volume rendering the mechanical mixing unfeasible. Most concave-up CSDs, regardless if they are interpreted as two segments or not, share similar slopes in the populations of smallest crystals, originating from the latest stage of crystallization. This supports similar limiting crystallization behavior across different magma pulses, which can be driven by common evolution of intensive parameters at the end of crystallization.

In this thesis, we implement three-dimensional numerical model for melt crystallization. The model provides quantitative textural data of simulated textures, which are comparable to those derived from natural samples and in turn enables determining the crystallization processes and conditions relevant to magmatic environment. Our results show that monotonous rates of nucleation and growth lead to the delayed increase of crystallinity and hence significant deviation from the equilibrium trends. The application of numerical models to the natural textures points to the role of heterogeneous nucleation and mechanical movement of crystals on their aggregation during crystallization of granitic magmas. Crystal size distributions from different textural types of granites indicate a common evolution of

crystallization environment during the end of the solidification, which reflects a common evolution of the intensive parameters in individual magma pulses forming a granitic suit. Numerical approaches *via* forward and inverse modeling of crystallization, along with testing of our models on the field data, thus enable to deepen and extent our understanding of crystallization processes in the Earth's crust by iterative fashion.