

## Anisotropic diffusion in crystals: Insights from computer simulations

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Trace element concentration profiles in natural crystals offer insights into their morphologic and thermal evolution. Analyses of core to rim traverses in single crystals often assume one-dimensional geometry and neglect the effect of variable diffusivity associated with crystal anisotropy. Here, we introduce a numerical model that explores the effects of anisotropic diffusion on the distribution of trace impurities in single crystals as they grow. After nucleation, each new layer introduces impurities to the system, while a diffusion process continually lowers the concentration. We consider the effects of changing growth rate ( $G$ ), initial impurity uptake concentration ( $U^0$ ), crystal geometry ( $\theta$ ), and diffusivity along two orthogonal crystallographic directions ( $\kappa_x$  and  $\kappa_z$ ). We solve the system for the two-dimensional case using a finite-difference scheme.

Our results demonstrate that crystals growing with a constant growth rate develop a homogeneous internal concentration ( $\Gamma^0$ ) that is dependent on each of  $G$ ,  $U^0$ ,  $\theta$ ,  $\kappa_x$ , and  $\kappa_z$ . Diffusion profiles evolve with time and are characterized by a boundary layer thickness ( $\delta$ ).

Results of the model reproduce the general trends of trace element concentration profiles observed in natural hydrothermal quartz crystals. Brazilian specimens show diffusion of trace hydroxyl species in profiles perpendicular to the  $c$ -axis that vary systematically with distance to the terminus. With increasing height, FTIR analyses show decreasing  $\Gamma^0$  and diffusion profiles with smaller  $\delta$ . These trends can be matched by simulations that involve changing growth rates during crystallization. Our model can be used to constrain the natural growth rates of these crystals and offer quantitative insights into the overall time involved in their growth. Our approach thus potentially offers a new method to constrain the lifetimes of natural hydrothermal circulation systems.

## Complete chemical characterization of metapelitic minerals from W. Maine, USA: petrologic implications

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Complete chemical characterization of a suite of rock-forming minerals in well-equilibrated metapelites of western Maine, USA provide an exceptional opportunity to investigate mineral chemical systematics in their petrologic context. An extensive collection (>600 samples) of metapelites covers the spectrum of metamorphic grades (chlorite through second sillimanite zone) under roughly isobaric conditions (~ 4 kbar) and have minerals with ranges of Mg-Fe contents largely due to variations in bulk compositions and influences of sulfide-silicate interactions. In order to reduce the compositional variables that may influence the minerals, samples are considered in terms of the presence of minerals that can act as saturating phases (e.g. ilmenite for Ti) and can act as general monitors of oxidation conditions (e.g. graphite or magnetite). This approach has led to determination of an isobaric Ti saturation surface for biotites from graphitic, peraluminous metapelites that contain ilmenite or rutile. This surface provides a basis for a Ti-in-biotite geothermometer and allows a way to evaluate Ti-substitution mechanisms in biotite.

More in-depth analyses have been carried out on a subset of these samples with the addition of H, Fe<sup>2+</sup>, Fe<sup>3+</sup>, and/or Li determinations on biotite, muscovite, tourmaline, chlorite, staurolite, garnet and ilmenite. Among other features, these data have allowed us to refine the nature of Mg-Fe<sup>2+</sup> partitioning among mafic minerals as a function of temperature (i.e. influence on exchange thermometers) and to demonstrate that there are distinct ranges of Fe<sup>3+</sup>/Fe<sub>total</sub> ratios for Fe-bearing minerals in equilibrium with graphite, ilmenite, magnetite and/or hematite. In turn, in the absence of Fe<sup>3+</sup> determinations, the presence of certain oxidation-monitor minerals can be used to infer likely Fe<sup>3+</sup> ratios in mafic minerals in other metapelites.