A MODEL FOR MULTICOMPONENT DIFFUSION IN IONIC CRYSTALS

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This contribution deals with diffusion in ionic crystals that are solid-solutions and feature more than two end-member components. The interdiffusion of ionic species is of crucial importance, e.g., for (1) assessing the preservation potential of growth zoning and element partitioning during changing P-T conditions and (2) diffusion-chronometry via analysis of secondary compositional zoning in minerals.

We theoretically address ionic diffusion in the situation when both *binary exchange* of cations between neighbouring lattice sites and *vacancy mediated self-diffusion* of cations are important. The model equations are derived from linking expressions for the system's free energy with Onsager type reciprocity relations. The resulting diffusion equations are non-linear: The diffusive flux of each component depends on the concentrations and concentration gradients of all components and, of course, on all self-diffusion and binary exchange coefficients. The dependence is neither postulated nor fitted, it is directly derived from the model.

The suggested model is solved numerically and is verified using experimental data for diffusion in the Na-^{39}K-^{41}K three-component system of isotopically doped alkali feldspar. Among other things, the model is applied for constraining the proportions among the self-diffusion coefficients of Fe, Mg, and Ca in garnet from complex secondary compositional zoning, as observed in partially resorbed garnet from a mafic granulite.