THEME 1: THE DYNAMIC SOLID

Session 1.4: Solid solutions

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Solid solutions are at the core of geochemistry, mineralogy and petrology and underpin the economic basis of many mineral deposits. Solid solution formation on surfaces is also an important metal uptake mechanism in environmental systems. One of the main handicaps in effective predictive modelling of such systems, is the absence of data on thermodynamic, physical and structural properties for solid solutions at a range of scales. The aim of the session is to present advances in this field, which include 1) new data on the nature of substitutions in specific solid solution systems and 2) new methods to study or model solid solution properties. The goal is to relate microscopic details of atomic interaction to macroscopic properties that can be applied to geochemical systems. The topics include direct experimental measurements, thermodynamic modelling, computer simulation of solid solutions at the atomic level, characterization of microscopic properties (by for example spectroscopy, TEM, X-ray diffraction, etc.) and definition of the thermodynamic and kinetic factors controlling ion partitioning between solids and fluids, including phase-equilibrium determinations, kinetics and non-equilibrium partitioning, reaction paths and compositional zoning patterns in crystallizing solids, non-equilibrium and self-organization phenomena, etc.

1.4.11

Model of oscillatory zoning in the $(Ba,Sr)SO_4$ solid solution system

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Many minerals in nature exhibit oscillatory zoning, whereby their chemical composition varies more or less regularly along a crystal core-to-rim profile. A well-known example of oscillatory-zoned crystals obtained in controlled laboratory conditions is found in the $(Ba,Sr)SO_4$ solid solution system. These crystals precipitate from counter diffusing aqueous solutions at room temperature. In this contribution, we present a model for the formation of oscillatory zoning in such binary solid solutions. The model combines diffusive transport with an autocatalytic continuous growth process. Linear stability analysis and numerical solutions confirm the existence of oscillatory Ba concentration profiles across the crystal. The effects of fluctuations in the aqueous solution concentrations are also considered. These effects include noise-induced oscillatory zoning. This model may be useful in understanding the formation of oscillatory zoning in hydrothermal environments.