



Towards a structure-based model for the thermodynamic properties of feldspars

Ross Angel (1), Lindsay Sochalksi-Kolbus (1), Nancy Ross (1), Mario Tribaudino (2), and Fabrizio Nestola (3)
(1) Dept. Geosciences, Virginia Tech, Blacksburg, United States (rangel@vt.edu), (2) Dipartimento di Scienze della Terra, Università di Parma, Italy, (3) Dipartimento di Geoscienze, Università di Padova, Padova, Italy

Feldspars are the dominant phases in the Earth's crust. Knowledge of their thermodynamic and elastic properties is therefore essential for understanding petrological processes, including phase transformations, chemical reactions and cation partitioning. However, the complex and often non-linear structural response of feldspars to changes in pressure, temperature, and especially composition (e.g. the plateau effect), invalidates the use of simple solution models to define the thermodynamic properties and elasticity of real minerals across both the dilute (trace element) regime and the bulk solid solutions. The answer is to develop models to predict the thermodynamic and elastic properties of mineral solid solutions based directly upon crystal chemistry and implicitly incorporate the atomic-scale mechanisms of the structural response of the mineral to changes in intensive thermodynamic variables.

We will present the results of our initial analyses that are the first steps in a long-term project to develop a structure-based model for feldspars. The model is based on the concept of characterizing the structural response not in terms of bond lengths and angles, but on the cooperative tilts of the relatively rigid tetrahedra that form the framework of feldspars. We will show that the rigid-unit deformations of the tetrahedral framework can be decomposed in to four tilts of the four tetrahedra that comprise the 4-rings that lie parallel to (010). We will show that within the alkali feldspars change in just one of these tilts is responsible for changes in the length of the feldspar crankshaft, and is thus responsible for 70% of the volume change of alkali feldspars with P, T, or X. This provides the structural mechanism to explain the observation that the thermal expansion of alkali feldspars scales with the room-pressure volume, and provides a way in which to predict the cation site sizes required for calculation of trace element distribution coefficients.

This work was supported in part by NSF grant EAR0738692 to NL Ross and RJ Angel.