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Thermoelastic and thermodynamic properties of plagioclase feldspars from thermal expansion measurements

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Abstract

Powder X-ray diffraction patterns between 90 and 935 K have been collected for nine plagioclase samples, with different compositions and degree of Al-Si order. The refined volumes have been modeled using the Wallace and Suzuki formulations based on the Mie-Grüneisen EOS. No significant difference has been found between the Suzuki and Wallace formulations, and between the Einstein and Debye approximations of lattice energy. A Wallace model with the first derivative of the bulk modulus constrained to the experimentally determined values leads to refined Grüneisen parameters between 0.49 and 0.41, without any definite trend between albite and anorthite; the Einstein temperature in intermediate plagioclase is $\theta_E \sim 650$ K, but it is lower in albite [$\theta_E = 453(5)$ K].

A good fit with experimental heat capacity data for the $An_{60}Ab_{40}$ composition has been found using two Einstein-like oscillators with $\theta_{E1} = 230(3)$ K and $\theta_{E2} = 952(7)$ K, $X_{\theta E1} = 0.391(5)$. The change with temperature in $An_{60}Ab_{40}$ of the Grüneisen parameter is small at $T > 150$ K, with a slight decrease with temperature. Similar results could be obtained by independent refinement of an Einstein model with two oscillators to the volume data for the same composition [$\theta_{E1} = 205(30)$ K, $\theta_{E2} = 873(52)$ K, and $X = 0.36(4)$].

The components of the thermal strain tensor with temperature have been calculated and confirm that the greatest deformation is along the **a*** axis, i.e., along the extension direction of the crankshaft chains of the feldspar structure. Anomalous behavior of the strain tensor components in the **a-c** plane has been observed in albite and $An_{27}Ab_{73}$, and is related to an increase in the *c* unit-cell parameter with decreasing temperature.

Keywords: Thermal expansion, plagioclase, low temperature, thermoelastic properties