American Mineralogist, Volume 83, pages 2–22, 1998

Calibration of excess thermodynamic properties and elastic constant variations associated with the $\alpha \leftrightarrow \beta$ phase transition in quartz

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Abstract

Spontaneous strains for the $\alpha \leftrightarrow \beta$ transition in quartz were determined from lattice parameter data collected by X-ray powder diffraction and neutron powder diffraction over the temperature range ~5–1340 K. These appear to be compatible with previous determinations of the order parameter variation in α quartz only if there is a non-linear relationship between the individual strains and the square of the order parameter. An expanded form of the 2-4-6 Landau potential usually used to describe the phase transition was developed to account for these strains and to permit calculation of the elastic constant variations. Calibration of the renormalized coefficients of the basic 2-4-6 potential, using published heat capacity data, provides a quantitative description of the excess free energy, enthalpy, entropy, and heat capacity. Values of the unrenormalized coefficients in the Landau expansion that include all the strain-order parameter coupling coefficients were used to calculate variations of the elastic constants. Values of the bare elastic constants were extracted from published elasticity data for β quartz. Calculated variations of C_{11} and C_{12} match their observed variations closely, implying that the extended Landau expansion provides a good representation of macroscopic changes within the (001) plane of quartz. Agreement was not as close for C_{33}, suggesting that other factors may influence the strain parallel to [001]. The geometrical mechanism for the transition involves both rotations and shearing of SiO_4 tetrahedra, with each coupled differently to the driving order parameter. Only the shearing part of the macroscopic distortions appears to show the same temperature dependence as other properties that scale with Q^2. Coupling between the strain and the order parameter provides the predominant stabilization energy for α quartz and is also responsible for the first-order character of the transition.