American Mineralogist, Volume 82, pages 213–244, 1997

REVIEW

Theory of displacive phase transitions in minerals

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ABSTRACT

A lattice-dynamical treatment of displacive phase transitions leads naturally to the soft-mode model, in which the phase-transition mechanism involves a phonon frequency that falls to zero at the transition temperature. The basic ideas of this approach are reviewed in relation to displacive phase transitions in silicates. A simple free-energy model is used to demonstrate that Landau theory gives a good approximation to the free energy of the transition, provided that the entropy is primarily produced by the phonons rather than any configurational disorder. The ''rigid unit mode'' model provides a physical link between the theory and the chemical bonds in silicates and this allows us to understand the origin of the transition temperature and also validates the application of the soft-mode model. The model is also used to reappraise the nature of the structures of high-temperature phases. Several issues that remain open, such as the origin of first-order phase transitions and the thermodynamics of pressure-induced phase transitions, are discussed.