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Elastic properties of clinopyroxenes: Nonlinear lattice elasticity at high-pressure transformations

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Since clinopyroxenes (cpx) are important phases of the Earth's crust and upper mantle, the polymorphism of cpx and and phase stabilities of the individual cpx polymorphs have been in the focus of several studies in order to understand the mechanical and acoustic properties of this major mantle constituent. An important issue is how the cation substitution influences both the elastic properties and the polymorphic transformations at nonambient P-T-conditions. Here we report on an experimental study focussing on changes of the lattice properties associated with the monoclinic-to-monoclinic and monoclinic-to-triclinic phase transitions in silicate cpx at high pressures. The in-situ investigations have been carried out using X-ray single-crystal diffraction and Raman spectroscopy based on the diamond-anvil high-pressure technique. All measurements were performed at hydrostatic conditions up to 10 GPa. The parameters for the crystallographic lattice geometries have been used to evaluate compressibility moduli below and above the critical transition pressure, according to fits of appropriate 2nd- and 3rd-order Birch-Murnaghan equations of state. Bulk moduli for volume compression, but also the compressional moduli of the length changes for the main lattice-vector directions, have been used to calculate the evolution of spontaneous strain for the lattice across the transition. The C2/c-to-P21/c transition in spodumene at 3.2 GPa reconfirms all features of previously reported elastic softening phenomena, i.e. the higher compressibility of the high-P phase and a larger dK/dP dependency above the transition (K = 154 GPa for P $<$ 3.2 GPa, K = 125 GPa for P $>$ 3.2 GPa). The equivalent phenomenum has been observed for the C2/c-P-1 transformation in Na-Ti-cpx (K = 126 GPa for P $<$ 4.4 GPa and K = 120 GPa for P $>$ 4.4

GPa), with a pronounced nonlinear evolution in all main lattice directions.