Effective pair potential for Ca-O bonds in CaGeO$_3$ perovskite, garnet, wollastonite

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The CaGeO$_3$ perovskite and garnet were synthesized in a cubic anvil type apparatus under high pressure. The measurements of Ca and Ge K-edge XAFS spectra were carried out in the transmission mode at temperature up to 700 K. The effective pair potentials $V(u) = au^2/2 + bu^3/3!$, for Ca-O bond in various phases of CaGeO$_3$ have been investigated by the temperature dependence of EXAFS Debye-Waller factors. The potential coefficient $a$ for the Ca-O bond in perovskite-type CaGeO$_3$ is small, 4.4 eV/A$^2$, compared with those in garnet (6.0 eV/A$^2$) and wollastonite (6.4 eV/A$^2$). The potential for Ca-O bond in perovskite is broader than those in other CaGeO$_3$ polymorphs, which is one reason for the Clausius-Clapeyron’s curve for perovskite-garnet phase boundary having a negative slope. The potential coefficients for the Ca-O in perovskite are significantly smaller than those for the longer Ge-Ge distances as the framework vibration though the potential coefficient decreases usually as a result of the larger bond distance.