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Effect of isovalent Si,Ti substitution on the bulk moduli of $Ca(Ti_{1-x}Si_x)SiO_5$ titanites

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Abstract

The equations of state of *A*2/*a* titanite phases of $CaTiSiO_5$, $Ca(Ti_{0.5}Si_{0.5})SiO_5$, and $CaSi_2O_5$ have been determined from high-pressure X-ray diffraction measurements. The isothermal bulk moduli are $K_{0,T}$ = 131.4(7) GPa (for $P > 3.6$ GPa), 151.9(1.6) GPa, and 178.2(7) GPa, respectively, for a second order Birch-Murnaghan equation-of-state (i.e., with $K' = \partial K/\partial P = 4$). Refinements of third order equations-of-state yielded values of K' that did not differ significantly from 4. The complete substitution of Si for Ti in the octahedral sites of the titanite structure, therefore, results in approximately a 30% increase in bulk modulus and a 13% increase in density. The large stiffening of the structure can be attributed to the absence of rigid-unit modes from the structure and the direct involvement of cation-cation interactions in the compression of the structure.