American Mineralogist, Volume 100, pages 215–222, 2015

Thermo-compression of pyrope-grossular garnet solid solutions: Non-linear compositional dependence

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Abstract

Unit-cell parameters of a series of synthetic garnets with the pyrope, grossular, and four intermediate compositions were measured up to about 900 K and to 10 GPa using synchrotron X-ray powder diffraction. Coefficients of thermal expansion of pyrope-grossular garnets are in the range 2.10–2.74 $\times 10^{-5}$ K^{-1} and uniformly increase with temperature. Values for the two end-members pyrope and grossular are identical within experimental error $2.74 \pm 0.05 \times 10^{-5}$ K^{-1} and $2.73 \pm 0.01 \times 10^{-5}$ K^{-1}, respectively. Coefficients of thermal expansion for intermediate compositions are smaller than those of end-members and are not linearly dependent on composition. Bulk modulus of grossular is K_0 = 164.3(1) GPa (with K_0' the pressure derivative of the bulk modulus fixed to 5.92) and bulk modulus of pyrope is K_0 = 169.2(2) GPa (with K_0' fixed to 4.4) using a third-order Birch-Murnaghan equation of state, which are consistent with previously reported values. The bulk moduli of garnets of intermediate composition are between ~155 and ~160 GPa, smaller than those of the end-members no matter which K_0' is chosen. The compositional dependence of bulk modulus resembles the compositional dependence of thermal expansion. Intermediate garnets on this binary have large positive excess volume, which makes them more compressible. We find that excess volumes in the pyrope-grossular series remain relatively large even at high pressure (~6 GPa) and temperature (~800 K), supporting the observation of crystal exsolution on this garnet join. The curiously "W"-shaped compositional variation of thermal expansion and bulk modulus is anti-correlated with the compositional dependence of microstrain documented in our companion paper (Du et al. in preparation) on the excess volumes in this series of garnets. Minimum thermal expansions and bulk moduli go with maximum microstrains.

Keywords: Pyrope-grossular garnet solid solution, thermal expansion, compressibility, excess volume