American Mineralogist, Volume 102, pages 184–191, 2017

Effect of composition on compressibility of skiagite-Fe-majorite garnet

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Abstract

Skiagite-Fe-majorite garnets were synthesized using a multianvil apparatus at 7.5–9.5 GPa and 1400–1600 K. Single-crystal X-ray diffraction at ambient conditions revealed that synthesized garnets contain 23 to 76% of an Fe-majorite component. We found that the substitution of Fe^{2+} and Si^{4+} for Fe^{3+} in the octahedral site decreases the unit-cell volume of garnet at ambient conditions. Analysis of single-crystal X-ray diffraction data collected on compression up to 90 GPa of garnets with different compositions reveals that with increasing majorite component the bulk modulus increases from 159(1) to 172(1) GPa. Our results and literature data unambiguously demonstrate that the total iron content and the Fe^{3+}/Fe^{2+} ratio in (Mg,Fe)-majorites have a large influence on their elasticity. At pressures between 50 and 60 GPa we observed a significant deviation from a monotonic dependence of the molar volumes of skiagite-Fe-majorite garnet with pressure, and over a small pressure interval the volume dropped by about 3%. By combining results from single-crystal X-ray diffraction and high-pressure synchrotron Mössbauer source spectroscopy we demonstrate that these changes in the compressional behavior are associated with changes of the electronic state of Fe in the octahedral site.

Keywords: Skiagite-majorite garnet, single-crystal X-ray diffraction, Mössbauer spectroscopy, equation of state, upper mantle, transition zone