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

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Garnets are among the most abundant phases in the upper mantle and transition zone; hence data on their behavior under extreme conditions is important for understanding the composition, structure, and dynamics of the deep Earth's interior. Natural garnets are usually complex solid solutions because the garnet structure can accommodate a number of different divalent and trivalent cations. While most cations in garnet occur in a single oxidation state ($Al^{3+}$, $Ca^{2+}$, $Mg^{2+}$, $Cr^{3+}$), iron commonly occurs as both $Fe^{2+}$ and $Fe^{3+}$. The major $Fe^{3+}$-bearing garnets are andradite ($Ca_3Fe_2Si_3O_{12}$), khoharite ($Mg_3Fe_2Si_3O_{12}$), and skiagite ($Fe_3Fe_2Si_3O_{12}$).

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. *[1] Ismailova et al. Am Min Volume 102, pages 184–191, 2017*