Mixing behavior between grossular and andradite: Evidences from X-ray diffraction and Raman spectrum

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Mineral inclusions in diamonds reflect the compositional features of the diamondiferous sources so that they can provide important information of the upper mantle and even the transition zone. Since Moore and Gurney (1985) [1] found majoritic garnet inclusions in kimberlitic diamonds, the majoritic garnet inclusions have become significant samples to understand deep earth processes. According to Kiseeva *et al.* (2018) [2], the majoritic garnet inclusions have a ferric iron fraction ($Fe^{3+}/\sum Fe$) increasing with depth. Recently, Xu *et al.* (2017) [3] discovered some majoritic garnets (from a depth of ~ 400 km) with ferric iron proportions as high as 0.81. In order to understand the origin of these Fe^{3+}-rich garnet inclusions, the physical-chemical properties of the Fe^{3+}-bearing garnets should be investigated. So far, no many studies have been carried out though.

In this study, we performed experiments to synthesize garnets with their compositions along the grossular-andradite binary at 3 GPa and 1100 - 1200 °C, in order to investigate the effect on the physical-chemical properties of replacing Al^{3+} with Fe^{3+} on the octahedral sites of the garnet. The synthetic samples were investigated by BSE, EMPA, powder XRD and unpolarized Raman spectroscopy. The garnets had grain sizes between 20 ~ 100 um as indicated by BSI, and had generally homogenous compositions as suggested by the EMPA data. Charge balance calculations showed that most garnets had ferric iron fractions exceeding ~0.95. With an approximately linear dependence of the lattice parameters on the composition, the volume-mixing behavior should be generally ideal. We collected multiple Raman spectra from each sample, and evaluated the effects of crystal orientation and compositional heterogeneity on the Raman peak positions. Relations between the garnet compositions and Raman peak frequencies were also analyzed. Most Raman modes show linear behavior across the binary, whereas some of them do not. The reasons have been explored.

According to the results of this study, we can infer that the elastic properties of the grossular-andradite binary might be linearly dependent to the composition. The Raman spectroscopic data are important for deriving some important thermodynamic data.

[1] Moore & Gurney (1985) *Nature* **318**, 553-555. [2] Kiseeva *et al.* (2018) *Nature Geoscience* **Volume 11**, 144-147. [3] Xu *et al.* (2017) *Science Advances* **3**, e1601589.