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Cation ordering, twinning, and pseudo-symmetry in silicate garnet: The study of a birefringent garnet with orthorhombic structure

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Abstract

The crystal structure of a birefringent garnet (~$Adr_{53}Grs_{47}$) that occurs as a late-stage rim on andradite from Stanley Butte, Graham County, Arizona is analyzed and refined using single-crystal XRD. The structure has an orthorhombic *I* 2/*a* 1 2/*d* (unconventional setting for *Fddd*) space group symmetry, with unit-cell parameters of $a = b = 11.966(3)$ Å, $c = 11.964(3)$ Å, $\alpha = \beta = 90°$, $\gamma = 90.29(2)°$, $V = 1713.0(7)$ Å^3, $Z = 8$. The orthorhombic garnet displays very high birefringence (δ ~0.021) produced by the strong Fe-Al ordering in the octahedral sites, with Fe occupancies of 0.804 and 0.221 in Y_1 and Y_2 sites, respectively. Diffraction peaks (such as 101 and 103) violating the $Ia\bar{3}d$ symmetry of cubic garnet are obvious even in powder XRD pattern. The homogenization temperatures of the fluid inclusions suggest that the low-crystallization temperature is responsible for the ordered orthorhombic structure. The strong ordering state of the structure and the sharp boundaries in the chemical zoning in the crystal (between ~$Adr_{53}Grs_{47}$ and ~Adr_{100}) indicate the orthorhombic intermediate grandite garnet is a thermodynamically stable phase at low temperature, separated by wide miscibility gaps from the pure end-members (grossular and andradite) with cubic structures. Most of the previously reported triclinic garnet structures are likely artifacts produced by pseudo-merohedral twinning of less-ordered orthorhombic structure, as indicated by the characteristic pairing pattern of different Y-sites with the same occupancies.

Keywords: Orthorhombic garnet, Fe-Al ordering, non-cubic garnet, birefringent garnet, pseudo-merohedral twinning, fluid inclusion