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Structure and twinning of tetragonal $Ca_3Mn_2Ge_3O_{12}$ garnet

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ABSTRACT

Single crystals of tetragonal $Ca_3Mn_2Ge_3O_{12}$ garnet (space group symmetry $I4_1/a$, a = 12.3098(7) Å, c = 12.3277(9) Å) were characterized by X-ray diffraction and transmission electron microscopy. Their structure is topologically isosymmetric to tetragonal high-pressure garnets such as majorite, displaying the same two distinct types of macroscopic twin mechanisms. Twinning occurs as pseudo-merohedral ferroelastic twin lamellae with preferred orientation of the twin-domain boundaries parallel to $\{101\}_{tet}$, whereas merohedral ferrobielastic twin domains occur without any orientational preference. The crystal structure was determined from single-crystal X-ray diffraction data of a crystal fragment completely free of pseudo-merohedral twin domains. It shows two different Jahn-Teller distorted MnO_6 octahedra, with a different orientation of the axis of polyhedral elongation. The ordering scheme of these Jahn-Teller distorted octahedra follows in an alternating pattern the densest rod packing, and the cooperative effect of the electronically induced octahedral distortion was found to be responsible for the cubic-to-tetragonal symmetry breaking in $Ca_3Mn_2Ge_3O_{12}$ garnet. The extent of polyhedral distortion indicates a partially dynamic character of the Jahn-Teller effect. The distortion of the tetrahedral T2 sites controls the cooperative effect of the lattice strain induced by the Jahn-Teller distortion of the Mn^{3+} octahedra and thus is responsible for the overall lower symmetry.