

Crystal structure of Guinier-Preston zones in orthopyroxene: Z-contrast imaging and ab initio study

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ABSTRACT

Nano-precipitates of Guinier-Preston zones (or G.P. zones) occur in slowly cooled orthopyroxenes (OPX). Due to their nanometer sizes and intergrowth with host OPX, both X-ray diffraction and high-resolution TEM imaging cannot provide a consistent structure model for the G.P. zone precipitates. Combining Z-contrast imaging and density functional theory (DFT) methods, a correct crystal structure for the G.P. zone precipitates can be obtained, because Z-contrast imaging can reveal positions and occupancies of atoms directly. The crystal structure for the G.P. zone has $P2_1/c$ symmetry with 4 types of tetrahedral chains (OA1, OA2, OB, OC). The structure can be considered as periodic stacking of half unit cells of enstatite sub-layers and of diopside sub-layers in a twinning-like relationship along a -axis. The G.P. zones that precipitate out from their host Ca-bearing OPX at low temperature are metastable with respect to end-members of enstatite and diopside.

Keywords: Orthopyroxene, diopside, G.P. zone, nanomineral, DFT, Z-contrast imaging, order-disorder, enstatite