American Mineralogist, Volume 83, pages 799–810, 1998

Distribution of cations and vacancies and the structure of defects in oxidized intermediate olivine by atomic-resolution TEM and image simulation

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ABSTRACT

The Fe, Mg, and vacancy distributions in oxidized olivine of intermediate composition and the crystal structures of associated planar defects were examined by a combination of atomic-resolution transmission electron microscopy, image analysis, and image simulation. Simulated images using various structures and site occupancies show that the defects are not laihunite-like layers within an essentially normal olivine, but instead are integral parts of a highly oxidized crystal with a high degree of cation and vacancy ordering and a distorted olivine structure. A possible new structure was derived as a variant of previously published refinements for oxidized fayalite (laihunite-3*M*), with one defect row per unit cell instead of two. Details in high-resolution images are extremely sensitive to variations in atomic positions and site occupancies. Semiquantitative constraints on relative magnitudes of electron densities provided by image simulation were combined with crystal chemical constraints based on local charge balance and compositional constraints from analytical electron microscopy in a series of linear equations, which were solved to provide several candidate models for the distribution of Fe, Mg, and vacancies. Simulations using the new structure and an occupancy model in which essentially all of the Fe is Fe^{3+} in M2 sites and all of the vacancies are in M1 sites match significant characteristics of HRTEM images obtained at Scherzer defocus and at overfocused conditions. This ordering scheme is similar to that of true laihunites and may result from differences in site and cation sizes.