American Mineralogist, Volume 90, pages 1256–1264, 2005

High-resolution transmission electron microscopy (HRTEM) study of the 4*a* and 6*a* superstructure of bornite Cu_5FeS_4

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ABSTRACT

The crystal structure and microstructure of bornite have been of great interest to mineralogists since the pioneering studies of Morimoto and his colleagues (Morimoto 1964; Koto and Morimoto 1975). Because many questions about bornite remain, we are re-examining its structure using HRTEM. High-resolution transmission electron microscope (HRTEM) images taken along the <101> axis of bornite and processed by CRISP show variations of contrast between superstructure images and sublattice (1*a*) images. This contrast variation in the processed images is assumed to arise from vacancy ordering. Atom coordinates in the 4*a*-I and 6*a*-I superstructures are determined with the assumptions that superstructures possess the same symmetry as the sublattice and metal atoms occupy tetrahedral sites. Final structural models of 4*a*-I and 6*a*-I superstructures are calculated using simultaneous equations involving structure factors derived from Fourier transforms (FT) of HRTEM images, and the results are confirmed by image and diffraction simulations. With these models, the non-systematic extinctions are explained by the statistical vacancy ordering patterns. However, due to various approximations, the structures proposed are only possible models, but not unique solutions. So far, no low-temperature structure of bornite (2*a*4*a*2*a*) has been observed, but 1*a*, 2*a*, and 4*a*-I or 6*a*-I superstructure domains are always found to coexist in bornite near room temperature. We have also found that electron beam damage can induce the 1*a*2*a*1*a* superstructure.