3-D Structure Determination of $CAMoO_4$ using HVEM

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The three-dimensional (3-D) structure of an inorganic crystal, $CaMoO_4$, was solved by electron crystallography utilizing the HVEM installed at the Korea Basic Science Institute (KBSI) in 2003. It has capability of high tilting ($\pm 60^o$) and atomic resolution (0.12 nm). HRTEM images from 4 different major zone axes and selected-area electron diffraction patterns from 18 different zone axes were obtained. The 3-D electron diffraction data resulted in the basic crystallographic information of $CaMoO_4$, space group $I4_1/a$, a = 5.29Å and c = 11.54Å. A crystallographic image processing (CIP) of HRTEM images was used to determine the atomic coordination of $CaMoO_4$.

The initial values of average phase errors (φ_{res}) for [001], [100], [110] and [111] HRTEM images were 14.1^o, 3.3^o, 7.7^o and 22.1^o, respectively. Further refinement of the structures was carried out using additional HRTEM images and electron diffraction patterns in different microscopic conditions. Effects of image quality, diffraction quality, specimen tilting, irradiation damage and energy filtering on the structure refinement have been evaluated.

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