

Incommensurate Modulated Structure Determination by Combining HREM and ED

Fang-hua Li, Hai-fu Fan, *Institute of Physics, Chinese Academy of Sciences, Beijing, China*. E-mail: lifh@aphy.iphy.ac.cn

The incommensurate modulated structure can be treated as a multi-dimensional (MD) periodic structure cut with a three-dimensional hyper plane^[1]. In the case of one-dimensional modulation the structural modulation reveals directly in the high-resolution electron microscope image projected in the direction perpendicular to the modulation wave vector, but the image resolution is usually insufficient for showing all atoms. In this work it is shown that the electron diffraction data can be utilized to enhance the determined structure resolution by means of the MD direct methods^[2].

The electron diffraction pattern consists of main reflections and satellites. The main reflections correspond to the average structure. An arbitrary defocus image is averaged according to the unit cell of basic structure to obtain the average image, and the deconvoluted average image reveals the average structure. Fourier transform of the deconvoluted average image yields phases of low-resolution main reflections for the modulated structure. Phases of high-resolution main reflections for the modulated structure can be derived from the low-resolution phases obtained from the image and the amplitudes from the diffraction pattern. The MD direct-phasing method^[2] can be used for phase extension and refinement of main reflections, and then used for phase extension from main reflections to satellite reflections.

[1] De Wolff P.M., *Acta Cryst. A*, 1974, **A30**, 777. [2] Hao Q., Liu Y.W., Fan H.F., *Acta Cryst.* 1987, **A43**, 820.

Keywords: incommensurate modulated structure, high-resolution electron microscopy, electron diffraction