11.7-5 SOLUTION TO THE X-RAY PHASE PROBLEM FOR ACENTRIC CRYSTALS. By S.L. Chang and J. A.P. Valladares, Instituto de Física, UNICAMP, Campinas, SP, 13100, BRASIL.

An experimental method to solve the X-ray phase problem for noncentrosymmetric crystals is developed, using Bragg-type three-beam diffraction. This method results from a consideration of the phase dependence of line profiles in 5-beam reflections for wavelength $\lambda$ above and below a critical absorption edge $\lambda_{\text{c}}$ of the heaviest constituent atom in the crystal. It is found that for $\lambda > \lambda_{\text{c}}$, the sign of the sine of invariant phase is a product of the signs defined from asymmetry of the line profile and the sense of rotation of the crystal lattice. Application of this method to several 3-beam cases shows an exact agreement between the experimentally determined phases and the theoretical ones. Comparison between this method and the previously proposed method for centrosymmetric crystals (Chang, Phys. Rev. Lett. 48, 163, 1982) is given.

Dynamical calculation has also been carried out to provide dispersion surface and diffracted intensities for Bragg-type and transmission-type multiple diffractions in centro- and noncentro-symmetric crystals. It is shown that the phase-dependent line-profile asymmetry is an effect due to total reflection in 3-beam Bragg-type diffraction and that the line-profile asymmetry of transmission-type diffraction fails to provide correct phase information.

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