

differences $|F^+|^2 - |F^-|^2$ cannot be measured, and only the intensities $I_h = |F^+|^2 + |F^-|^2$ are experimentally available; b) dispersive differences between $(|F_2^+|^2 + |F_2^-|^2)$ and $(|F_1^+|^2 + |F_1^-|^2)$ may be estimated from the experiment, however the estimates may be heavily affected by the casual and/or by the systematic overlapping present in the diffraction patterns. The evident minor experimental information provided by a powder diffraction experiment discouraged the use of MAD and its applications up to now. This new approach combines the joint probability distribution function method with MAD techniques to solve the phase problem from powder data. The probabilistic bases of the method were established and the distributions are calculated by assuming the prior knowledge of the scattering intensities I_h collected at two wavelengths, the first close to the absorption edge of the anomalous scatterer and the second far away from it. The method is able to derive from these quantities the formulas providing estimates of the substructure structure factor moduli $|F_o|$ which allow to retrieve the anomalous scatterer positions by means of Patterson deconvolution or Direct Methods [1]. Given the anomalous scatterer substructure the method leads to formulas estimating the full structure phases and their reliability [2]. The related procedure was implemented into a modified version of EXPO2004 [3]. Applications to synchrotron data will be shown.

[1] Altomare et al., **2009**, *J. Appl. Cryst.* 42, 30-35. [2] Altomare et al., **2009**, *Acta Cryst.* Submitted. [3] Altomare et al., **2004**, *J. Appl. Cryst.* 37, 1025-1028.

Keywords: anomalous dispersion; powder data; structure solution

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The Indicator - Reflexes and Influences of Various Factors on Their Intensity. Mahmud G. Kyazumov^a.

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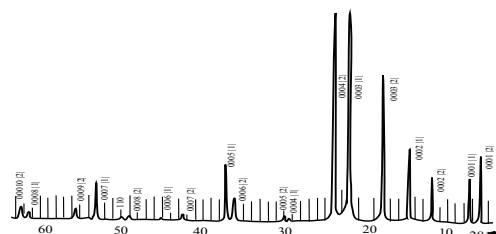
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On diffraction patterns the indicator-reflexes (IR) pointing to the types of packages which form crystal structures of many layered semiconductors have been revealed. It has been established that the magnitude l of the strongest reflex in the series $000l$ for hexagonal and $00l$ for monoclinic structures and also of the second strong reflex in the series $hh2hl$ ($h=\text{const.}$) for hexagonal and $0kl$ ($k=\text{const.}$) for monoclinic structures defines quantities of filled by cations the polyhedral (T and O) layers in the cell and points to the TOTE, TOTTE, TOOTE, TTOTTE, TOTE0OE, TOTE0OETOTE types of packages. Where T is the tetrahedron, O is the octahedron, E is the empty layer.

The research of influence of various factors on the intensity of IR results in the use of these reflexes as the indicator of quality.



Fig 1. Electron diffraction pattern of 2H polytype of CdInGaS₄ monocrystal with TOTE type packet.



The figure 2 demonstrates the powder X-ray diffraction of GaFeS_{2.7}, where layered microcrystals are oriented parallel to substrate. The 0003 [1] peak indicates first TOTE phase with the parameters of lattice $a=3,653\text{\AA}$ and $c=12,033n\text{\AA}$, and the 0004[2] peak indicates TOTTE phase with the parameters of lattice $a=3,653\text{\AA}$ and $c=14,868n\text{\AA}$, where n is the quantity of layers in polytypes.

Keywords: diagnostics; diffraction data; layered compounds

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Powder Neutron Diffraction of Hydrogenous Materials-What is Possible Today? Marc Schmidtman^a, Chick C. Wilson^a, Valeska P. Ting^b,

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Understanding structure–property relationships plays a key role in current material science research and hydrogen is undoubtedly a key element to a wide range of materials. The accurate structural determination of hydrogen, however, is at least difficult and often impossible with current experimental methods. One experimental method, powder neutron diffraction (PND) was long perceived as inapplicable for hydrogenous materials due to the large incoherent scattering contribution of the ¹H nucleus – thus the determination of hydrogen has been a particular problem when the naturally abundant ¹H