

change in the interplanar spacings  $\Delta d/d, d(x)$  and so on). The  $\Delta(\vec{a})$  is distributed to Fisher. The  $\Delta(\vec{a})$  is defined by the expression:

$$\Delta(\vec{a}) = \frac{N-M}{M-1} \sum_{k=1}^M N_k f_k^{-1} (\bar{\xi}_k - \hat{c} f_k^T(\vec{a}_k, \vec{a}))^2 / \sum_{k=1}^M N_k \sum_{j=1}^{N_k} f_k^{-1} (\xi_k^j - \bar{\xi}_k)^2$$

where  $N = \sum_{k=1}^M N_k$  - a full number of measurements,  $\hat{c}$  - parameters  $c$  value, that minimizes

$$S(c) = \sum_{k=1}^M N_k \left( \bar{\xi}_k - c f_k^T(\vec{a}_k, \vec{a}) \right)^2$$

for any  $\vec{a}_k : N_k$  - number of measurements,  $\xi_k^j$  - result of the  $j$ -th measurement,  $f_k \sigma^2$  - dispersion of measurements error,  $\sigma^2$  - unknown parameter,  $f_k$  - an unknown true value of measurement, which can be good estimate by the mean value  $\bar{\xi}_k = \sum_{j=1}^{N_k} \xi_k^j \cdot N_k^{-1}$ ,  $f_k^T(\vec{a}_k, \vec{a})$  - is

a theoretical value for the fixed vector  $\vec{a}$ . We analyse the confidens set  $D$ , whose elements are vectors  $\vec{a}$ , for which take place inequality  $\Delta(\vec{a}) \leq F_{M-1, M-M, \alpha}$  ( $\alpha$  - the given confidence level). The problem of the confidence intervals construction can be solved by the simple sorting of the vectors  $\vec{a}$  values near  $\vec{a}_{min}$ , which minimizes  $\Delta(\vec{a})$ . For a small number of the model parameters the problem is stable. When the number is large, it is necessary to make use of the regularizing algorithms (Tikhonov A.N. et al. Regulariziruju - shtchije algoritmy i apriornaja informatsija. Moscow, Nauka PH, 1983, p.195).

11.7-16 EFFECTS OF WEAKLY EXCITED REFLECTIONS ON THE TWO-BEAM CASE OF DYNAMICAL X-RAY DIFFRACTION. By H. K. Wagenfeld, Royal Melbourne Inst. of Technology, Melbourne, Australia, and H. J. Juretschke, Polytechnic Inst. of New York, New York, USA.

Bethe(1928, Ann. Phys.,Lpz. 87,55) formulated the dynamical theory of electron diffraction for a two-beam case and included weakly excited additional reflections by adding perturbation terms in the potential. A systematic extension of this method to x-rays, including coupling of the two polarizations (Juretschke, 1984, Acta Cryst., to be published) can be used to predict changes in two-beam properties caused by additional reflections, for Laue and Bragg cases. Hart and Lang (1961, Phys. Rev. Lett. 7,120) showed that Pendellosung fringe spacings are changed to an Aufhellung by the excitation of extra reflections. This change in spacing follows directly from the changes in effective structure factor and in the absorption coefficient of the standard two-beam interaction predicted by the theory for this four-beam case.

11.7-17 X-RAY STANDING WAVE MEASUREMENTS OF NONCENTROSYMMETRIC STRUCTURES) By M. Bedzyk and G. Materlik, Hamburger Synchrotronstrahlungslabor HASYLAB, Hamburg, Germany.

When diffracting an x-ray plane wave from a single crystal, the diffracted and incident traveling plane waves interfere to form a standing wave-field. As is known, the phase of this interference pattern relative to the diffraction planes is a function of the Bragg reflection angle.

For a noncentrosymmetric Bragg reflection from a III-V single crystal, the position of the diffraction planes relative to the atomic lattice depends on the x-ray scattering factors  $f(\vec{H})$  of the two different atomic species. Due to anomalous dispersion, this diffraction plane position is in turn dependent on the x-ray energy. As an example, with respect to the corresponding centrosymmetric position, the (111) noncentrosymmetric diffraction planes are shifted in the [111] direction by an amount:

$$\Delta(111) = \frac{1}{8} + \frac{1}{4\pi} \left[ \tan^{-1} \left( \frac{f_V^0 + f_V^I + f_{III}^{II}}{f_{III}^0 + f_{III}^I - f_V^{II}} \right) + \tan^{-1} \left( \frac{f_V^0 + f_V^I - f_{III}^{II}}{f_{III}^0 + f_{III}^I + f_V^{II}} \right) \right],$$

where  $f = f^0 + f^I + f^{II}$ . ( $f^I$  and  $f^{II}$  are the anomalous dispersion corrections.) In an x-ray standing wave measurement the position, of either one of these two atoms, relative to the diffraction planes can be determined and used to calculate the noncentrosymmetric shift  $\Delta(\vec{H})$ . By using the energy tunability of the x-ray standing wave instrument installed at the Hamburger Synchrotron Radiation Laboratory, it was possible to measure the energy dependence of  $\Delta(111)$  in the vicinity of the respective K absorption edges for a GaAs(111) single crystal.

11.7-18 POLARIZATION-MIXING OF X-RAYS (QUANTUM THEORY OF INTERFERENCE OF WHITE X-RAYS). By T. Ohkawa and H. Hashimoto\*, The Institute of Vocational Training, Sagami-hara city, Kanagawa, Japan,\*) Department of Applied Physics, Osaka University, Suita, Osaka, Japan.

X-ray polarization effect has been a vexing problem which has recently been given serious interest, however conventional theoretical predictions have failed to explain the origin of the rotation of polarization direction. In order to study the mechanism of the polarization of x-rays in crystal, relativistic quantum field theory is applied to the process of x-ray diffraction. Two photon state is theoretically investigated for analysing the mechanism of the polarization-mixing. This theoretical method is also applicable to discuss the resonative interference of white x-rays of proximate energy. The Feynman's graphical method is employed to expand the 2nd order perturbation, in which inner photon-line of quantum theoretical concept is introduced which is assumed to have analogical meaning to Ewald's "Winnen Welle" that travels in the crystal field with radiationless dipolewave. The conventional structure factor has been expanded with static electron's distribution, however to discuss the interference phenomena taking place in atomic field, dynamic nature of electron's behaviour is necessary to incorporate, so that dispersion relation of diffracted x-rays similar to Laue's dynamical theory is shown by use of scattering S-matrix. Dynamical structure factor is defined on the base of Dirac's matrix.