II. REAL AND IDEAL CRYSTALS

11.8-03 NEW DEVELOPMENTS IN EXTINCTION CORRECTIONS. CONNECTION WITH PHYSICAL PROPERTIES. By P. Becker (1), F. Dunstetter (1), P. Bastie (2), H. Germani (3)

1. CNRS, 25 rue des Marois, 75015 Paris Labor. Cristallographie, co 140 54373 Nancy Cedex
3. Labor. Crist. co 140 54373 Nancy Cedex

I. Decomposing the entrance surface of the crystal into a superposition of point sources, it is possible to calculate exactly the X-ray or neutron integrated power for a rectangular crystal. This allows a comparison with approximate treatments, and modification of those proposed. It is also possible to compare the results with the model of H. Fano. The case of perfect crystals will also be discussed.

II. Variation of Gamma ray intensities in KDP and RbDP with temperature, around the ferroelectric transition, has shown the possibility of reproducing data assuming a mosaic spread of the form: a + b/(T - Tc).

A thermodynamic model, of Landau's type, allows one to prove that the ratio a/b is correct physically, and this opens new types of application.

III. In polarized neutron experiments, when the Bragg vector is not perpendicular to magnetization, one has to consider the scattering process where spin is reversed. We propose an exact matrix solution, and an approximate expression for correcting for this effect. Applications will be presented.

III. Decomposing the entrance surface of the crystal into a superposition of point sources, it is possible to calculate exactly the X-ray or neutron integrated power for a rectangular crystal. This allows a comparison with approximate treatments, and modification of those proposed. It is also possible to compare the results with the model of H. Fano. The case of perfect crystals will also be discussed.

II. Variation of Gamma ray intensities in KDP and RbDP with temperature, around the ferroelectric transition, has shown the possibility of reproducing data assuming a mosaic spread of the form: a + b/(T - Tc).

A thermodynamic model, of Landau's type, allows one to prove that the ratio a/b is correct physically, and this opens new types of application.

III. In polarized neutron experiments, when the Bragg vector is not perpendicular to magnetization, one has to consider the scattering process where spin is reversed. We propose an exact matrix solution, and an approximate expression for correcting for this effect. Applications will be presented.

11.8-04 THE SATELLITE POSITIONS IN THE BRAGG CASE. By I.R. Entin and K.P. Asur

Institute of Solid State Physics, USSR Academy of Sciences, 142432, Chernogolovka, Moscow district, USSR.

The kinematic expression for an angle between satellites occurring in the vicinity of the diffraction reflex H when exciting in the crystal an ultrasonic wave with a wave vector

\[ \mathbf{k} \parallel \mathbf{H} = \Delta \mathbf{k}_s \cos \theta_s \] (1), \( \theta_s \) the wave number of the incident radiation. In the Bragg case when \( k_s \) is sufficiently small the satellites should have occurred within the total reflection region which is obviously devoid of any physical sense. The limitation of the kinematic approach to the problem was remarked by Hapechev et al. (Kristallografiya 24, 430, 1979). Dynamical consideration consists in constructing a dispersion surface for a crystal with superlattices (I.R. Entin, Sov. Phys. JETP 50, 110, 1979). The self-intersections of the dispersion surface correspond to the centres of the satellites. The satellite width is determined by the width of the gap appearing with lifting of the degeneracy (Fig. 1b). At a small sound amplitude we have

\[ \Delta \mathbf{k} = \Delta_k^2 + \Delta_0^{1/2} \] (2) instead of (1), \( \Delta_k \) is the width of the total reflection region.

Deviations from the kinematic formula are connected with the fact that in the vicinity of Bragg reflection the effective refractive index is a function of the angle of incidence. Astrophil double-crystal technique was used in the experiment (Fig. 1b). On the rocking curve ((220) Si, AgK\(_{\lambda_1}\), Fig. 2a—without sound, Fig. 2b—longitudinal vibrations with the frequency \( \nu = 166.4 \text{ MHz} \) the satellites are positioned on the edges of the Bragg peak (\( \Delta \approx 2\Delta_0 \)) while \( \Delta \approx \Delta_0 \). When \( \Delta \approx \Delta_0 \) it follows from (2) that \( \Delta = \Delta_0 \) in accordance with the experimental result. When \( F \) dynamical consideration leads to the same expression as the kinematic consideration does, however satellites occur only with \( F_s \gg 1 \), \( z \) the extinction length. The width of the satellites (Fig. 3) (KDP, AgK\(_{\lambda_1}\), transverse vibrations, \( \nu = 209.5 \text{ MHz} \) is essentially smaller than the width of the principal reflexion and is determined by the vibration amplitude.

11.8-05 EXPERIMENTAL DETERMINATION OF EXTINCTION IN BERYLLIUM. By G. Spazzini, Department of Physics, University of Helsinki, Ciba-Geigy Laboratory, 20 D, Helsinki 17 Finland.

The theory of extinction is formulated in terms of directly observable quantities. The intensity coupling between the direct beam and the diffracted beam is called secondary extinction, and this effect is recovered from the reduction of the intensity of the direct beam when diffraction takes place. The reduction of the reflectivity per unit path length, \( \alpha \), due to the coupling of the amplitudes of the direct wave and the diffracted wave is called primary extinction. This depends on the correlation distance \( r \) of the crystal planes, when \( r \) is measured in units of the extinction length, \( (\lambda/V)c\beta \), where \( \lambda \) is the X-ray wavelength, \( r_0 = a^2/\lambda c \) the electron scattering length, \( c \) the polarization factor (1 or cos2) and \( F \) the structure factor of a unit cell of volume \( V \). At small enough values of \( r \) the primary extinction factor \( y = \alpha/(\text{kinematical}) = \exp(-r/2\lambda^2) \), and \( r \) can be determined by varying one of the factors \( \lambda, c \) or \( F \) and measuring the corresponding \( y \). The measurements were made on a slab of a single crystal in the symmetrical Laue geometry with X-ray polarized by a Bormann-polarizer. The requirements of negligible divergence and wavelength dispersion could be realized only for the case \( c = 1 \), and in the case \( c = 2/3 \) the correction for secondary extinction was found through an iterative procedure involving the assumption that \( y \) is a constant over the profile. Reflections (10-0), (00-2) and (10-1) were measured at many points over the crystal face, and \( c \) (kinematical) for each reflection was found by an extrapolation to \( r = 0 \). The resulting values of the structure factors \( F(10-0) = 1.8526.04, F(00-2) = 3.2020.05 \) and \( F(10-1) = 1.7260.04 \) indicate large anisotropy of the electron distribution of the Be atom in solid.