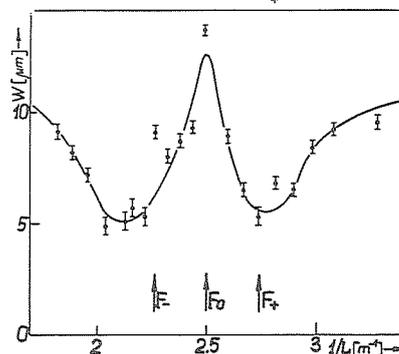


**11.5-09** THE DEBYE-WALLER FACTOR DUE TO STATIC DISPLACEMENTS AROUND HYDROGEN IN NIOBIUM. By H. Behr, H. Metzger and J. Peisl, University of Munich, W. Germany

H dissolved in Nb in the high temperature  $\alpha$ -phase will decrease the Bragg intensity due to static displacements of the Nb atoms from their average lattice sites (static Debye Waller Factor (DWF)). The relative integrated intensity of Bragg reflections from single crystals NbH<sub>x</sub> has been measured. The corresponding static DWF was found to decrease with the concentration ( $x < 0.2$  H/Nb) and the order of the reflection, as predicted by theory. For small scattering-vectors the static DWF is primarily determined by the displacements of the Nb atoms closest to the H impurity. Therefore the attenuation of the low order Bragg reflections was used to determine the displacements of these Nb atoms ( $u = 0.083 \pm 0.009 \text{ \AA}$ ). The measurement of the static DWF seems to be a simple and useful method for the determination of displacements close to impurities and other lattice defects.

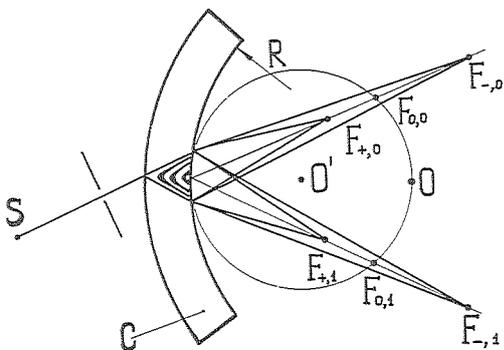
$$\frac{\cos \theta}{L} - \frac{1}{R} = \pm K(t/\Lambda) \cdot \frac{J_h}{2t \sin^2 \theta}$$

where L is the distance from the crystal, R is the bending radius, t is the thickness of the crystal,  $\Lambda$  is the extinction length,  $J_h$  is the Fourier component of the crystal polarizability,  $\theta$  is the Bragg angle. The computer calculation of the intensity distributions in the focusing region shows that the sharp dynamic focuses  $F_+$  and  $F_-$  must appear near the stationary phase points, but the coefficient  $K(t/\Lambda) \sim 1.22-1.27$  must be introduced into the focusing condition to take into account the cylindrical aberration. To avoid the chromatic broadening of the focus, both monochromatization of the radiation and the double-lens achromatic scheme were used. It was established that the diffracted beam is exposed to the dynamical contraction in the two regions near the calculated points to the width of  $W \sim 5 \mu\text{m}$  (fig.2) that is an order less than the Borrmann delta base ( $80 \mu\text{m}$ ).



**11.6-01** EXPLORATION OF THE DYNAMICAL DIFFRACTION FOCUSING OF X-RAYS BY THE HOMOGENEOUSLY BENT CRYSTAL. By V.I.Kushmir and E.V.Suvorov, Institute for Solid State Physics, Academy of Sciences of the USSR, Chernogolovka Moscow district, 142432, USSR.

The schemes of the dynamical focusing of X-rays by the homogeneously bent crystal stand out of all the theoretically studied schemes of the dynamical focusing owing to their characteristics because only in these schemes the magnifying coefficient k differs from unity and the resolution (when  $k > 1$ ) or the focus size (when  $k < 1$ ) must be about 1000-100 $\text{\AA}$ . The scheme of the cylindrical reducing lens was studied (fig.1).

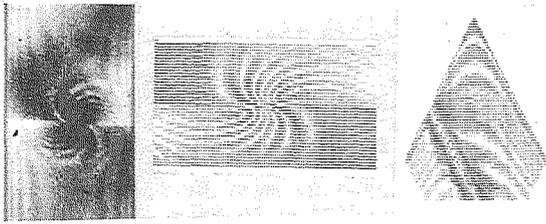


It was shown that the two stationary phase points corresponding to the two types of the Bloch waves in the crystal exist in both the direct and diffracted beams. The focusing condition is as follows:

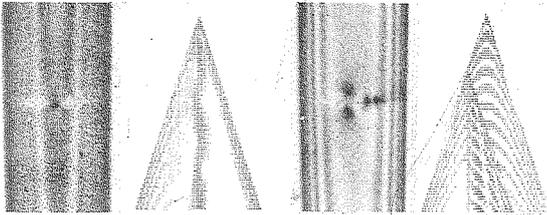
**11.6-02** X-RAY DISLOCATION CONTRAST By E.V.Suvorov, V.L.Indenbom and K.Yu.Mukhin, Institute of Solid State Physics, Academy of Sciences of the USSR, 142432 Chernogolovka Moscow district, USSR and Institute of Crystallography, Academy of Sciences of the USSR, Moscow

The diffraction mechanisms forming the X-ray image of the dislocations were studied. It was established that the mechanisms determining the formation of the image in the short-range and long-range dislocation fields have different physical nature. While the geometrical optics turned out to be convenient for the description of the formation of the long-range dislocation field image, the phenomena taking place in the short-range field demand the employment of the Bloch waves diffraction optics terms for their analysis. When exploring the dislocation images it was found that they may be formed due to a great variety of effects such as: interference of the Bloch waves coming along different trajectories, closeness and rarefaction of the beams, tilt of trajectories near the crystal surface, interference of the wave fields of different origin, interbranch scattering, waveguide effects, channeling, reflection and etc. The mechanisms were studied of formation of the votrex-like dislocation image that occurs on the high-order reflection topographs. It was found that the image in this case is formed as a result of the "new-born" and "old" wave fields interference and is a specific hologram of the elastic dislocation field obtained on the Bloch waves in the crystal. The experimental topograph, the computer-calculated section topographs and the

distribution of the wave field in the scattering plane are shown on fig.1.



It was experimentally revealed that the short-range dislocation field may develop the properties of a semiopaque mirror and even a waveguide. The topographs and correspondent computer-calculated intensity distributions illustrating the waveguide effect and the reflection of the Bloch waves from the short-range dislocation field are shown on fig.2.



**11.6-03** POLARIZATION STATES OF THE DYNAMICALLY DIFFRACTED X-RAYS IN THE LAUE CASE. By S. Annaka, Tokyo University of Mercantile Marine, Koto-ku, Tokyo, Japan.

Polarization states of the dynamically diffracted X-rays were analysed in the Laue-case 220 reflection of Si. As the  $\sigma$  state and the  $\pi$  state components of the electric vector of diffracted X-rays have different wavelengths in crystals, the phase difference between the two coherent components is produced depending on the crystal thickness. Accordingly the elliptically polarized X-rays or the rotation of the electric vector is expected for the linearly polarized incident beam. Using the conventional X-ray sources (Cu K $\alpha$ ) and the grooved Ge monochromator, the linearly polarized and horizontal X-ray beam was produced with the electric vector inclined at 45° to the horizontal plane. The X-ray beam had the  $\sigma$  and  $\pi$  components for the 220 Laue-case reflection of Si with the horizontal plane of incidence. The polarization states of the 220 reflection beam were analysed using the 333 reflection of Ge. The analysis was done mainly for the crystals about 55, 79 and 96  $\mu$ m thick respectively.

The experimental results suggested the polarization state, which was due to the phase difference of about  $\pi$ ,  $3/2 \pi$  and  $2\pi$  respectively between the  $\sigma$  state and the  $\pi$  state waves, corresponding to the above three cases of thickness. As there are four coherent waves with different absorption coefficients the resultant electric vector is not simple as in the optical case. It must be also considered in the interference that the shape of the intrinsic rocking curve is different for the two polarization states respectively.

**11.6-04** NONLINEAR TRANSFORMATION OF RADIATION FREQUENCY ACCOMPANIED BY DIFFRACTION IN CRYSTALS. By V.A. Belyakov & N.V. Shipov, All-Union Research Institute of Physical-Technical & Radiotechnical Measurements, Moscow, U.S.S.R.

Nonlinear transformation of electromagnetic radiation frequency in crystal is theoretically investigated. It is shown that essential enhancement of the nonlinear frequency transformation occurs if it is accompanied by diffraction of the generated radiation in the crystal.

The phase-matched second- and higher-harmonic generation is examined in detail for the case of the harmonic diffraction in the plane-parallel crystal plate. It is found that the nonlinear frequency transformation enhancement occurs for the case of Bragg diffraction and is due to an unusual dependence of the harmonic intensity on the sample thickness  $L$ . Instead of the common  $L^2$ , dependence of the harmonic intensity may be proportional to  $L^4$  if the diffraction takes place. At the maximum of enhancement the harmonic intensity is  $(FL/\lambda)^2$  times higher than in absence of diffraction, where  $\lambda$  is the harmonic wavelength,  $F$  is dimensionless structure amplitude of the relevant reflection, which for X-rays is typically  $\sim 10^{-5}$ .

This maximum may be achieved if the frequency of the phase-matched generated harmonic coincides with the edge of strong diffraction scattering (Edge of stop band). The value of the possible enhancement of the frequency transformation is reduced as  $|\lambda - \lambda_e|^{-1}$  if the harmonic wavelength  $\lambda$  (or the direction of its propagation) departs from the stop band edge  $\lambda_e$  and the enhancement vanishes if the corresponding departure (relative wave length change or angular decline) is greater than  $F$ .

It is noted that a special relation between the dielectric frequency dispersion  $d$ ,  $F$  and the Bragg angle  $\theta$  must be fulfilled for the maximum enhancement (e.g. for  $\theta = \pi/2$ ; the corresponding relation is  $F \approx d$ ).

The above enhancement relates to monochromatic waves, because the harmonic intensity oscillates with change of wavelength (or propagation direction) and the enhancement corresponds to the oscillation maxima which are divided by the intervals  $\Delta\lambda/\lambda \sim F^{-1}(\lambda/L)^2$ . This is the reason why the full strength of enhancement may be observed for well monochromatized and collimated beams. The averaging over the harmonic frequency line width and angular divergence of the beam reduces the observable enhancement. If the frequency line width  $\Delta\lambda/\lambda \geq F^{-1}(\lambda/L)^2$  the averaged over line width intensity of the harmonic  $I_\alpha$  is given by the expression  $I_\alpha = I_0(F\lambda_e|\lambda - \lambda_e|^{-1})^{1/2}$ , where  $I_0$  is the intensity of harmonic being generated in absence of diffraction.

The perspectives of an experimental observation of the nonlinear frequency transformation enhancement are discussed. As the most favorable the structures with large scale periodicity are named (e.g. cholesteric liquid crystals, incommensurate crystal structures and so on) for which the enhancement effect may be investigated by means of now available sources of coherent radiation.