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NOTE

A SIMULATION OF SECTION TOPOGRAPHS USING SYNCHROTRON RADIATION

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A section topography using synchrotron radiation is proposed and incidental problems are discussed with the aid of a computer simulation. The effect of higher order diffractions is examined for (111) and (110) systematic reflections, and it is shown that only a single reflection contributes to a topograph if we use an adapted wave length. The effect of a broad spectrum of the incident beam is also examined. Contribution to the images due to wave length extended up to $\pm 5\times 10^{-4}$ nm from a given wave length of 0.1 nm is inquired, and no troublesome effect is found.

Key words ; X-ray topography, synchrotron radiation, computer simulation.

1. Introduction

Because of its outstanding properties, such as a continuous wave length spectrum and high intensity, many X-ray diffraction experiments using synchrotron radiation have already been performed in various fields[1]. In Japan The Photon Factory in The National Laboratory for High Energy Physics is now under construction, and we can perform X-ray experiments in a few years[2].

Though the atomic arrangement surrounding a dislocation in solids with simple atomic structure is well known, that in solids with more complicated atomic structure is scarecely known. Recentry the authors reported topographs of dislocations in an ADP crystal[3] and expected that more detailed studies may give some information on the ionic arrangement surrounding them. As we suppose several dislocations ar-

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range themselves in some tens of micrometers, the section topography may be the only method to take the expected information. The section topography is believed to reveal most precise feature of defects and is readily compared with simulated images using a spherical wave theory which is capable of predicting numerically the intensity profiles of the outgoing beams[4)~9)].

In this note a section topography utilizing a continuous wave length spectrum of synchrotron radiation is proposed and assumed problem incidental to this method are discussed using simulated topographs. The simulation is made on a silicon crystal containing a dislocation in a Laue case using the computer program DEF 47 developed by Y. Epelboin[8)9)].

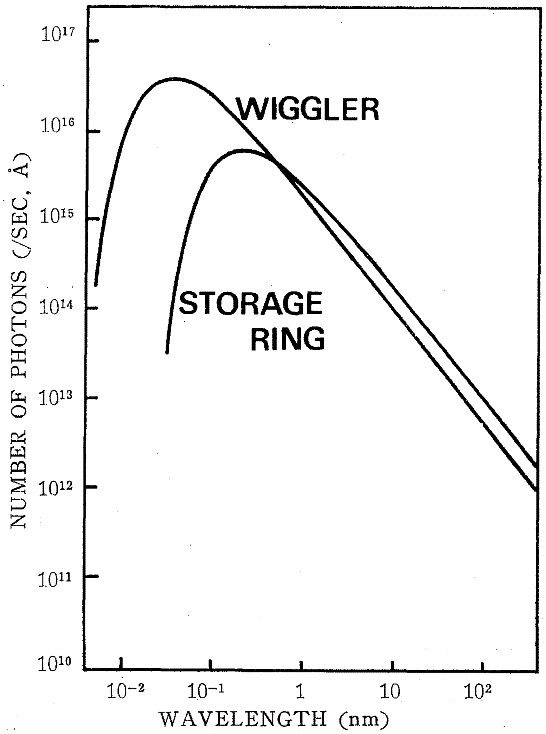


Fig. 1 Continuous wavelength spectra of The Photon Factory[2)]. The curve storage ring is the spectrum operated at 2.5 GeV and 0.5 A and the curve wiggler is that operated at the same condition but with wiggler.

2. Section topography using synchrotron radiation

The electromagnetic radiation emitted when a relativistic electron is accelerated in a synchrotron is a continuous wave length spectrum extending from 0.01 nm X rays up to visible light and has high intensity in X-ray range, more than a hundred times of X rays generated by rotating anode X-ray source. Owing to these outstanding properties application to X-ray topography is quite useful. The spectral distribution of intensity of the radiation is calculated correctly and that of The Photon Factory under construction is shown in Fig. 1[2]. The lower curve represents the spectrum expected in a 2.5 GeV and 0.5 A operation and the upper that expected installing the wiggler in the same operating condition.

Application of synchrotron radiation has already been made by Tanner *et al.*[10] or Tuomi *et al.*[11] and they used transmission pattern of Laue spots which correspond to conventional projection topographs. We propose a section topography with collimated X rays and have to examine the effects of continuous wave length precisely. The following two effects are examined with a computer simulation; 1) the effect of overlapping of images due to higher order reflections onto the image which is recorded by a given monochromatic wave length and 2) the the effect of overlapping of images due to a little shorter and/or longer wave lengthes caused by broad spectrum of incident beam onto the given image. For the collimation the slit system proposed by Hart[12] which is made by a set of lead, iron and aluminum may be installed.

Table 1 Relative intensities of higher order reflections (last column) for (111) and (110) systematic reflections. $I_h/P(\lambda)$, the fourth column is calculated by eq.(1). Correction for air absorption (fifth column) and sensitivity factor for emulsion (sixth column) are considered.

hkl	λ(Å)	ϑ°	$I_h/P(\lambda)$	$I_h/P(\lambda)\exp(-25\mu_{air})$	film	%
111	1.000	9.2	2249	2076	0.50	99.66
333	0.333	9.2	52	52	0.05	0.25
444	0.250	9.2	23	23	0.03	0.08
555	0.200	9.2	6	6	0.02	0.00
777	0.143	9.2	1	1	0.01	0.00
220	1.000	15	1020	1013	0.50	98.14
440	0.500	15	87	86	0.10	1.67
660	0.333	15	16	16	0.05	0.16
880	0.250	15	5	5	0.03	0.03

We choose (111) and (220) reflections of silicon crystal as given reflections and relative intensities of higher order reflections are calculated as shown in Table 1. We adapted 0.1 nm for the given reflection.

The absorption correction for air is taken from International Tables for Crystalloraphy with λ^3 interpolation. The sensitivity factors for Ilford L4-25 μm nuclear emulsions are refered to Hart[12]. The intensity I_h recorded on the emulsion due to the diffracted beam from a reciprocal lattice vector $\boldsymbol{h}$ is

$$I_h/P(\lambda) \propto F_h \cdot \lambda^3 \cdot \mathrm{cosec}^2 \vartheta_B \tag{1}$$

where $P(\lambda)$ is the incident intensity at wave length λ, F_h the structure factor and ϑ_B the Bragg angle for the given reflection. In the table the (111) reflection contributes 99.7% of the total diffraction intensity in the (111) systematic reflection, and (220) reflection contributes 98.1% of the intensity in the (110) systematic. While Hart[12] examined the (111) systematic reflection for wave length extending from 0.05 nm up

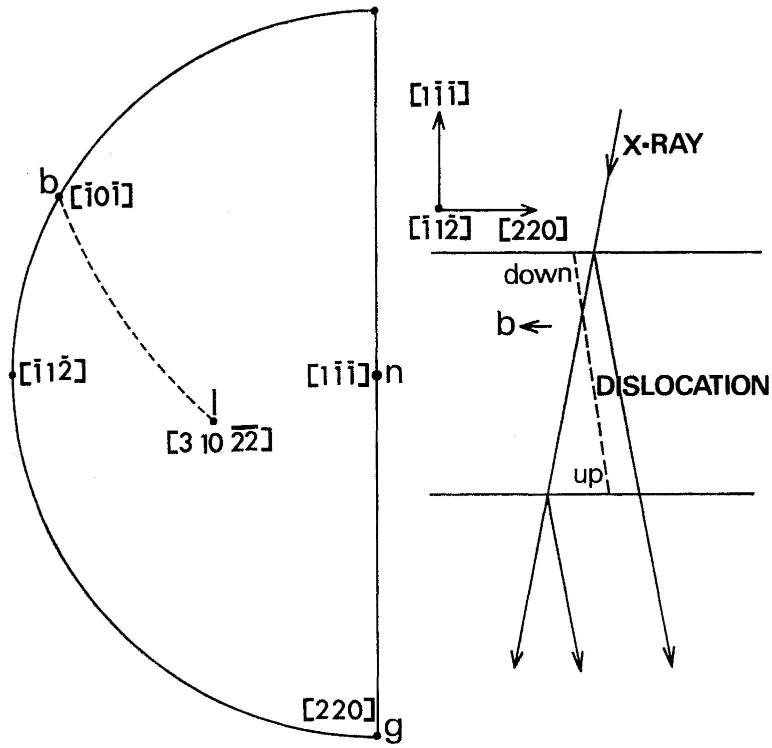
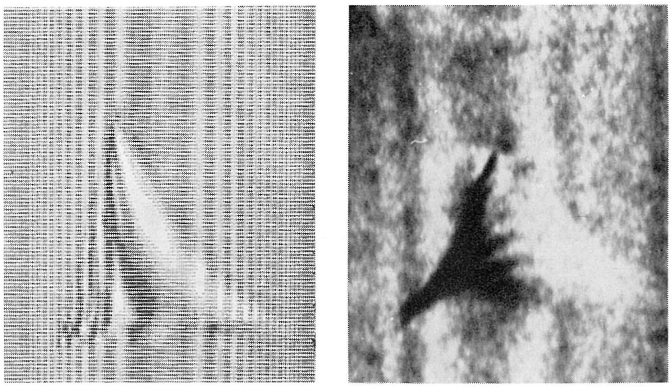


Fig. 2 Geometry to simulate section topographs. A 60° dislocation nearly parallel to one of the extreme side of the Borrmann fan runs downwards from the exit surface to the entrance surface of X rays. Dislocation line is along $\boldsymbol{l}$ with Burgers vector $\boldsymbol{b}$, and normal of crystal surface and diffraction vector are $\boldsymbol{n}$ and $\boldsymbol{g}$ respectively.



(a) (b)

Fig. 3 Correspondence of simulated topograph (a) with experimental section topograph (b). High-intensity direct and white dynamical images, and intermediate image which gives a fringe pattern are observed similarly.

to 0.5 nm and showed (333) and (444) reflections contribute 62% and 22% of the total intensity, respectively. Diffraction of long wave length is absorbed well in air and is prevented from reaching to emulsion, while that of short wave length is scarecely absorbed in emulsion, it is possible, then, to adapt an appropriate diffraction condition so that only the given reflection contributes to topograph.

3. Computer simulation

Takagi[4] has shown that the integrated intensity along the exit surface of a crystal may be calculated from the knowledge of the repartition of intensity along this surface. Epelboin[8] has developed a numerical methods of integrating the Takagi-Taupin equations. We simulate section topographs for a silicon crystal containing a dislocation using the computer program DEF 47 developed by Epelboin[9], which may be refered to the appendix. The pattern of a section topograph depends on a diffraction condition to take topograph and a geometry of dislocation line in the sample crystal, which are shown in Fig. 2. A 60° dislocation nearly parallel to one of the extreme side of the Borrmann fan runs downward from the exit surface to the entrance surface of X rays. Crystal surface is (111) and line direction and Burgers vector of dislocation are [3, 10, 22] and [101] respectively. Simulation is made with diffraction vector, [110]. Figure 3 is an example to show a correspondence of simulated topograph with experimental section topograph. In both topographs sample thickness, $t \sim 1/\mu$ and MoKα_1 radiation are used, where μ is a linear absorption coefficient of silicon. Geometrical condition for the section topograph may slightly different from the simulated one. In both topographs high-intensity direct and white dynamical images, and intermediate image which gives a fringe pattern are observed similarly.

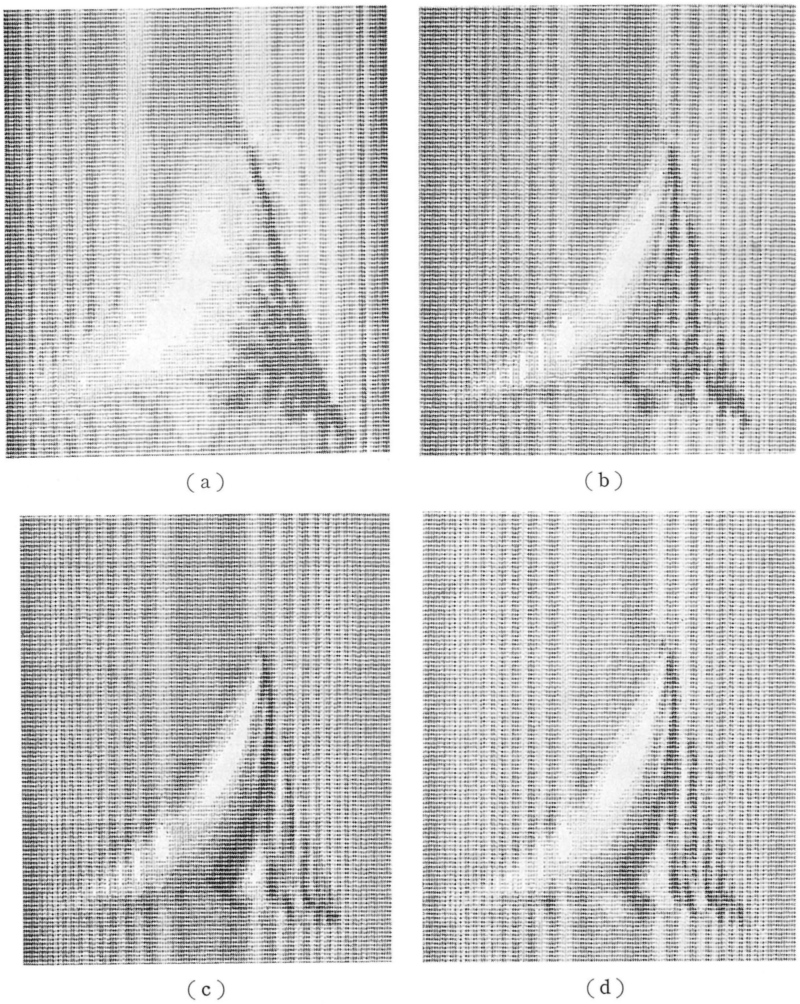


Fig. 4 Synthesized topographs to examine the effect of overlapping of images due to higher order reflections. Only the spectrum of incident beam is considered in (a) and (b), and correction for air absorption and sensitivity factors for emulsion is also considered in (c) and (d). Curve wiggler and storage ring in Fig. 1 is used for (a), (c) and (b), (d) respectively. Section topograph of given reflection is refered to Fig. 5(c).

4. Examinations with simulated topographs

Simulated topographs are made for (220), (440), (660) and (880) reflections for the same reflection angle and an expected topograph to examine the effect 1) is synthesized from them. The intensity of (220) reflection is extremely strong in (110) systematic reflection as shown in Table 1. The spectral distribution of intensity shown in Fig. 1 is not considered in the table. Figure 4(a) and (b) are synthesized taking

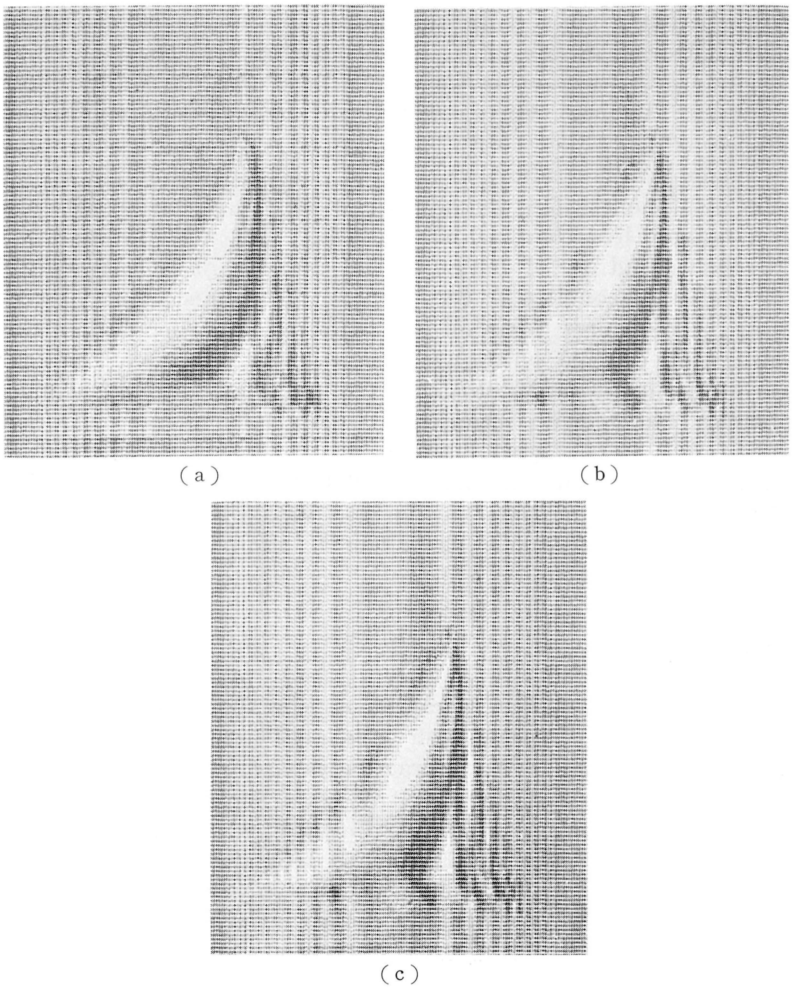


Fig. 5 Synthesized topograph to examine the effect of broad spectrum of incident beam. Wavelength at half-maximum is taken to be 0.1 ± 0.005 nm or 0.1 ± 0.0005 nm in (a) and (b) respectively. Main image of given reflection is (c).

only the spectrum into consideration, while (c) and (d) are synthesized taking not only the spectrum but correction for air absorption and sensitivity factors for emulsion into account. In Fig. 4(a) and (c) the curve wiggler in Fig. 1 is used and in Fig. 4(b) and (d) the curve storage ring is used. In Fig. 4(a) the effect of the shortest wave length dominates the topograph. The section topograph of given reflection is refered to Fig. 5(c). Comparing Fig. 5(c) with Fig. 4 we note some remarks. As the conventional nuclear emulsion scarcely absorb X rays shorter than 0.05 nm the effect of these rays is negligible. It is quite difficult to distinguish Fig. 4(d) from Fig. 5(c), so that we may overcome the difficulty caused by the effect 1). It appears that the best choice of the wavelength for a given reflection is those ranging at left shoulder of the curves. To use shorter wavelength it is necessary to develop new emulsions.

The monochromatization of X rays by the diffraction in sample crystal is insufficient. The wavelength at half-maximum of diffracted X rays is estimated less than ± 0.005 nm. The (220) topographs are simulated for wavelengthes of 0.1 ± 0.005 nm and 0.1 ± 0.0005 nm as well as for 0.1 nm, corresponding to the main image. The latter pair corresponds to the difference between Kα doublet. An expected topograph to examine the effect 2) is synthesized from three images. Two sub-images due to a shorter and a longer wavelength are overlappedon to the main image. The relative intensity of sub-images to the main image is taken to be one half. Figure 5(a) and (b) are synthesized topographs which wavelength at half-maximum are 0.1 ± 0.005 nm and 0.1 ± 0.0005 nm respectively. Comparing these topographs with Fig. 5(c) we can find no differences in their patterns. The effect 2), then hardly contributes to synthesized topograph.

5. Conclusion

Some incidental problems to take a section topograph using synchrotron radiation are discussed with simulated topographs. It is shown that the effect of higher order diffraction is effectively diminished adapting an appropriate wavelength. It is also shown that the effect of broad spectrum of incident beam is not important. Before taking section topograph using synchrotron radiation we have to develope collimating apparatus and/or goniomator stage which can be controlled remotely. If we must install a monochromator before sample crystal we can not expect strongly diffracted X rays.

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Appendix

Takagi has developed a dynamical theory which include any small distortion inside the crystal extending the conventional dynamical theory[4]. He showed X-ray intensity at a point on the exit surface can be calculated either by the method of Riemann function or by successive numerical calculations at each mesh point. Taupin uses a Ronge-Kutta nethod to calculate the intensity numerically[5]. This method is precise but needs computer time. Epelboin developed numerical methods of integrating the Takagi-Taupin equations in shortest computer time[8].

The intensity at a point on the exit surface of the crystal is calculated by a numerical integration of the Takagi-Taupin equations. The amplitudes of both refracted and reflected waves $\boldsymbol{D}_0$ and $\boldsymbol{D}_h$ are given by

$$\frac{\partial}{\partial s_0}\boldsymbol{D}_0(\boldsymbol{r}) = -i\pi K\chi_{\bar{h}}\boldsymbol{D}_h(\boldsymbol{r})$$