The Intensity Patterns with a Multi-Crystal Diffractometer Observed at a Synchrotron Source

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The intensity is calculated employing the expressions developed for a multi-crystal diffractometer. Comparison with the measurements shows the reliability of the formalism and enables better interpretation of the experimental results.

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Multi-crystal diffractometers are becoming increasingly employed for high resolution diffraction studies. The use of perfect crystals as optical components in these diffractometers is particularly suited for intense synchrotron radiation sources (SRS) with a highly collimated X-ray beam, where the dynamic scattering produces high peak reflectivity and a small angular range of diffraction. The obtained high resolution can be used for the characterization of epitaxial structures, surfaces, phase transitions or weak diffuse scattering avoiding the interference from the strong Bragg reflection. It is clear that the understanding of the intensity distribution around the Bragg reflections is essential for a reliable interpretation of the experiments and their optimization.

Considering an optical system with m monochromator components and n components for the analysers the intensity distribution can be described by a convolution integral extending the expression obtained for the triple-crystal diffractometer [1]:

$$I(\Delta\psi, \Delta\phi)$$
$$= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} J(\Delta\lambda)\, F(\alpha)\, R_{M_1}(\Delta\theta_{M_1})\, R_{M_2}(\Delta\theta_{M_2}) \cdots$$
$$\cdots R_{M_m}(\Delta\theta_{M_m})\, R_S(\Delta\theta_S)\, R_{A_1}(\Delta\theta_{A_1}) \cdots$$
$$\cdots R_{A_n}(\Delta\theta_{A_n})\, d\alpha\, d\lambda, \qquad (1)$$

where M, S, and A denote monochromator, sample and analyser, respectively. The intensity distribution around a reciprocal lattice point is measured by performing angular rotation $(\Delta\psi)$ of the sample and $(\Delta\phi)$ of the analyser. $J(\Delta\lambda)$ is the wavelength distribution around the characteristic line λ_0 and $F(\alpha)$ describes the spatial distribution of the emitted radiation of the source. The general expressions [2] for dispersive and
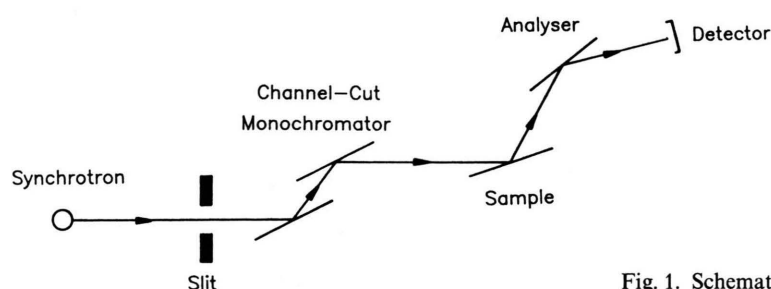

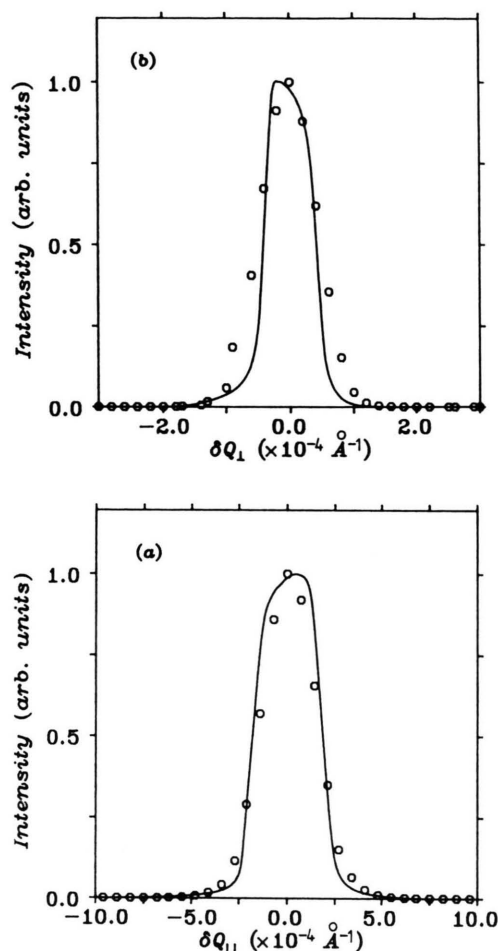Fig. 1. Schematic diagram of the diffractometer at the SRS.

Fig. 2. Theoretical and measured intensity profiles for the Si (400) Bragg reflection. a) parallel and b) perpendicular to the wavevector transfer $\bar{Q}$.

non-dispersive arrangements were derived for the angular deviations $\Delta\theta_{M_i}$, $\Delta\theta_S$, and $\Delta\theta_{A_i}$ from the Bragg condition at each of the crystal components of the ray with the wavelength $\lambda_0 + \Delta\lambda$ with respect to the ray of the nominal wavelength λ_0.

The calculations performed for the symmetrical (400) Si Bragg reflection were compared with the measurements [3] at the Daresbury SRS for an optical system consisting of a channel-cut Si double monochromator and Si single bounced analyser, both aligned for the symmetrical (111) Bragg reflection as shown in Figure 1. The Si sample, adjusted for (400) Bragg reflection, was aligned with the surface normal [100] and the direction [011] lying in the scattering plane. The premonochromator collimation corresponded to $1.3 \cdot 10^{-5}$ rad, and $J(\lambda)$ was taken as a
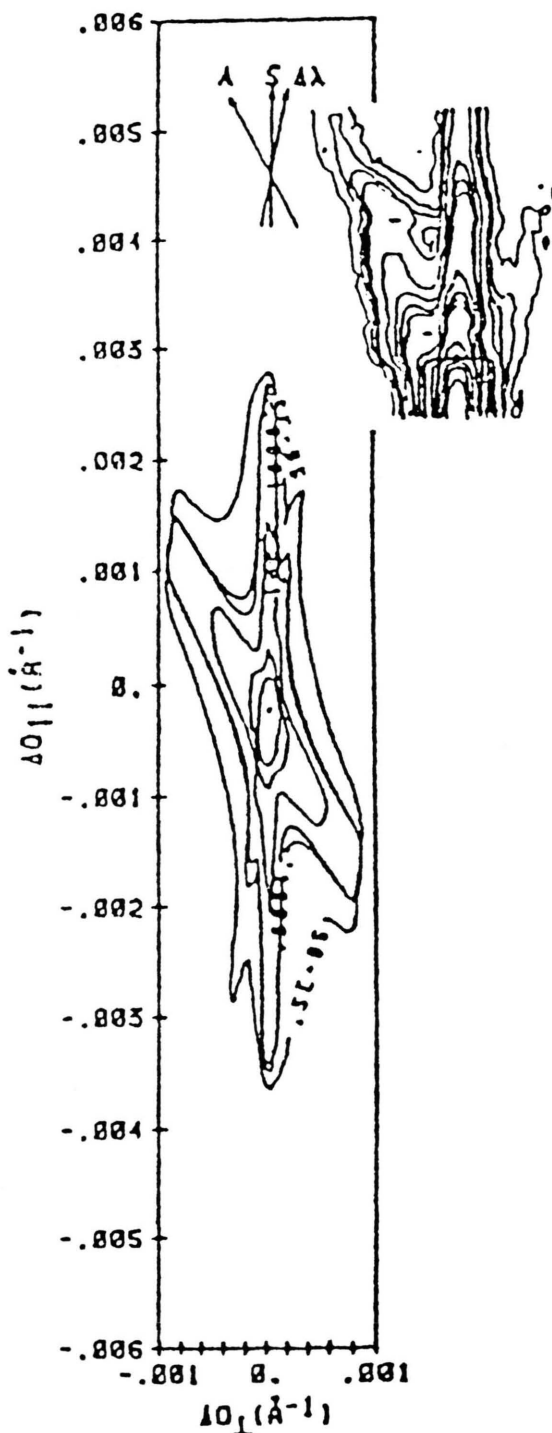

Fig. 3. Simulated intensity pattern around Si (400) Bragg reflection. The inset shows the measured pattern at the SRS. A, S, and $\Delta\lambda$ denote the analyser, surface and wavelength dispersion streaks, respectively.
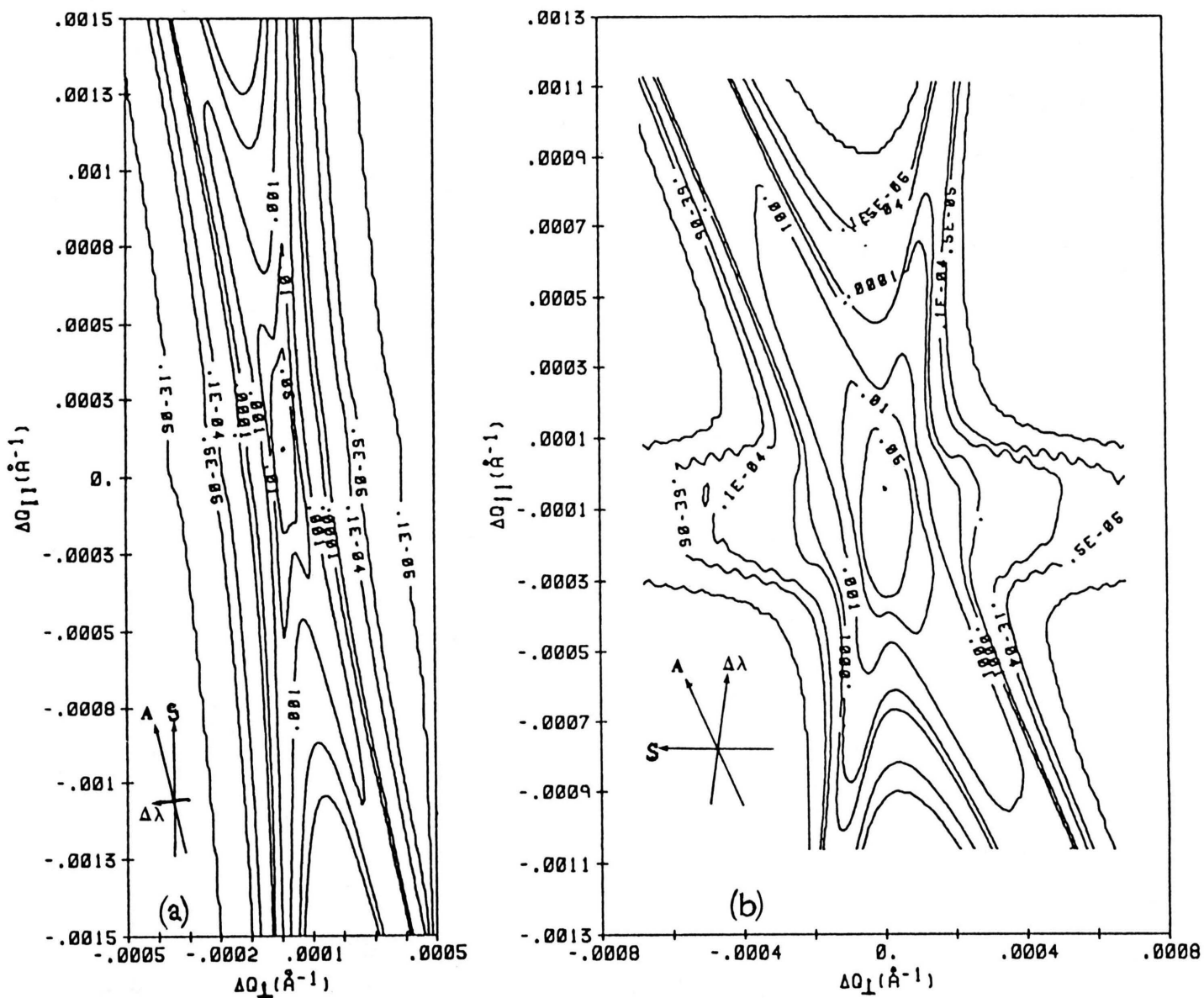
Fig. 4. Simulated intensity patterns a) around (111) InP symmetrical Bragg reflection and b) around (022) Si symmetrical Laue reflection. Notations as in Figure 3.

constant around the incident wavelength $\lambda_0 = 1.38$ Å. As can be seen in Fig. 2 the theoretical intensity profiles are in good agreement with the ones measured parallel ($\Delta Q_\parallel$) and perpendicular ($\Delta Q_\perp$) to the wavevector transfer. The simulated intensity distribution shown in Fig. 3 differs from the one obtained with a triple-crystal diffractometer at the conventional source [1]. The pattern is asymmetric since the double monochromator suppresses the monochromator streak. Also a weak wavelength streak $\Delta\lambda$ can be seen separated from the surface streak S. This effect is observed in the measurement with the synchrotron radiation because of its highly collimated incident beam, and it is shown in the inset in Figure 3. It follows from (1) that the $\Delta\lambda$ streak occurs at an angle $\tan^{-1}[\tan\theta_A \tan\theta_S/(2\tan\theta_S - \tan\theta_A)]$ to the wavevector transfer. Thus the $\Delta\lambda$ streak can become perpendicular to the wavevector transfer when $2\tan\theta_S$

$= \tan\theta_A$. This effect is calculated for an InP sample in symmetric (111) Bragg reflection with the InP monochromator and analyser aligned for the symmetric (222) reflection. The resulting weak $\Delta\lambda$ streak is shown in the simulated pattern in Figure 4a. The intensity distribution calculated for a sample in Laue (transmission) geometry is shown for the symmetrical (022) Si reflection. For samples with small absorption parameter μt as for Si, a strong surface streak S is expected perpendicular to the wavevector transfer as can be seen in Fig. 4b, where the directions of the analyser and $\Delta\lambda$ streaks are indicated in the inset.

In conclusion, it can be stated that the formalism developed for the multi-crystal X-ray diffractometer can provide an adequate description of the intensity distribution enabling better understanding and optimization of the experiments.

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[2] E. L. Gartstein and R. A. Cowley, Acta Cryst. **A 46**, 576 (1990).

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