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Increasing the size of search fragments for use in Patterson method calculations – the partial fragment rotation function. Erratum.

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Abstract

Equations given by Wilson [*Acta Cryst.* (1988) A44, 478-481] are corrected. There are misplaced brackets in equations (1) and (3) and an incorrect lower summation limit in equation (3).

Equation (1) should read

$$\sigma(\theta_1, \theta_2, \theta_3) = \sum_{\mathbf{h}} |F_{\mathbf{h}}^s|^2 \left[\left(\sum_i \cos 2\pi \mathbf{h} \cdot \mathbf{r}_i \right)^2 + \left(\sum_i \sin 2\pi \mathbf{h} \cdot \mathbf{r}_i \right)^2 \right] \quad (1)$$

and equation (3) should read

$$\sigma(\theta_1, \theta_2, \theta_3, \theta_p) = \sum_{\mathbf{h}} |F_{\mathbf{h}}^s|^2 \left[\left(\sum_{i=1}^{n_1} \cos 2\pi \mathbf{h} \cdot \mathbf{r}_i \right)^2 + \left(\sum_{i=1}^{n_1} \sin 2\pi \mathbf{h} \cdot \mathbf{r}_i \right)^2 \right] + \sum_{\mathbf{h}} |F_{\mathbf{h}}^s|^2 \left[\left(\sum_{j=n_1+1}^{n_2} \cos 2\pi \mathbf{h} \cdot \mathbf{r}_j \right)^2 + \left(\sum_{j=n_1+1}^{n_2} \sin 2\pi \mathbf{h} \cdot \mathbf{r}_j \right)^2 \right]. \quad (3)$$

All relevant information is given in the *Abstract*.

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Synchrotron X-ray diffraction on a CaF_2 microcrystal with 2·2 cubic micrometres volume.

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Abstract

The photon flux generated by the six-pole wiggler at CHESS combined with a focusing mirror and a focusing monochromator allowed diffraction experiments at 1·56 Å wavelength with a 2·2(5) μm^3 CaF_2 single crystal. The crystal was oriented by means of a multiwire proportional area counter. Reflection profiles and Bragg intensities were collected with a scintillation counter. The Bragg intensities were used for a structure refinement. The results demonstrate that crystals composed of light elements with volumes down to only 0·5 μm^3 can be mounted and used for single-crystal X-ray diffraction experiments. Until now such crystals have been considered as powder grains. Besides the possibility of applying single-crystal methods to materials of which larger crystals are not available the essentially extinction-free data from microcrystals allow a high-precision determination of electron densities and vibrational amplitudes.

Synchrotron radiation allows experiments on very small single crystals because of the low divergence and high brilliance of the beam. This feature stimulated experiments with a 200 μm^3 CaF_2 microcrystal (Bachmann *et al.*, 1983) and an 800 μm^3 zeolite microcrystal (Eisenberger, Neusam, Leonowicz & Vaugham, 1984). Rocking curves and reflection intensities have been recorded for these microcrystals. The Bragg intensities measured from the 200 μm^3 CaF_2 crystal have also been used for structure refinements and analyses of the mosaic spread of the crystal (Bachmann, Kohler, Schulz & Weber, 1985; Höche, Schulz, Weber, Belzner, Wolf & Wulf, 1986). Microcrystals of about 10^4 μm^3 volume have been used recently for diffraction experiments with macromolecular materials (Andrews, Papitz, Blake, Helliwell & Harding, 1988).

From the viewpoint of an X-ray scattering experiment the size of a crystal provides only a very rough estimate of the expected scattering effect, which is a function of the scattering power of a single crystal. The scattering power may be defined for an ideally imperfect crystal as

$$S = (F_0/V_e)^2 V_c \lambda^3 \quad (1)$$

where F_0 is the number of electrons per elementary cell, V_e and V_c are the volumes of the elementary cell and of the crystal, and λ is the wavelength. Usually crystals with $S = 10^{16}$–10^{17} are used for standard structure investigations. The above-mentioned CaF_2 (Bachmann *et al.*, 1983) and zeolite (Eisenberger *et al.*, 1984) microcrystals had scattering powers of $1{\cdot}45 \times 10^{14}$ and $1{\cdot}85 \times 10^{15}$, respectively.

Microcrystals with diameters smaller than the extinction length L behave as ideally imperfect crystals. The extinction

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