SHORT COMMUNICATIONS

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Rotation of spherical harmonics. Erratum.

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Abstract

An error in equations (3*b*) and (3*c*) of Su & Coppens [*Acta Cryst.* (1994). A**50**, 636–643] is corrected. The correct equations are

$$\alpha = \begin{cases} \arccos(R_{31}/\sin\beta) & \text{if } R_{32}/\sin\beta \geq 0 \\ 2\pi - \arccos(R_{31}/\sin\beta) & \text{if } R_{32}/\sin\beta < 0 \end{cases}, \quad (3b)$$

$$\gamma = \begin{cases} \arccos(-R_{13}/\sin\beta) & \text{if } R_{23}/\sin\beta \geq 0 \\ 2\pi - \arccos(-R_{13}/\sin\beta) & \text{if } R_{23}/\sin\beta < 0 \end{cases}. \quad (3c)$$

All relevant information is given in the *Abstract*.

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Friedel's law and non-centrosymmetric space groups.

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Abstract

It is shown that, in projections of non-centrosymmetric space groups having symmetry *p*3*m*1 or *p*31*m*, loci exist along which Friedel's law is obeyed even in the presence of n-beam interactions and phenomenological absorption. This theoretical prediction is verified by means of convergent-beam electron diffraction experiments on $Li_2ZnTi_3O_8$.

1. Introduction

Amongst the symmetry elements, the centre of inversion is well known to play a special role in electron scattering by crystals. For instance, where the kinematical description is a useful approximation, only the Laue groups can be determined unequivocally. Effects due to n-beam scattering in general are required to resolve this problem (Goodman & Lehmpfuhl, 1968). The analysis of non-centrosymmetric diffraction patterns, however, still presents particular difficulties. For certain non-centrosymmetric space groups, a simplification that can be utilized in initial interpretation is that, in the seven-beam approximation, zone-axis patterns reduce to an equivalent two-beam form (Moodie & Whitfield, 1994). It is now shown that, for specific space groups, loci exist along which Friedel's law is obeyed even in the presence of n-beam interactions. These serve to direct attention to specific areas in convergent-beam diffraction patterns where the failure of Friedel's law can be interpreted in structural terms.

Friedel's law states that the intensities of diffracted beams related by a centre of inversion are equal, that is, that $I(\mathbf{g}) = I(\bar{\mathbf{g}})$. When this is true, the space group of a crystal can be determined at best to within a centre of symmetry and this imposes a severe limitation on diffraction techniques.

The law is known to fail when absorption is significant or when dynamical scattering is strong. Bijvolet's method, of particular importance in the X-ray crystallography of organic materials, exhibits the first condition whilst convergent-beam electron diffraction is well suited to utilize the second condition.

In convergent-beam electron diffraction (CBED), loci are very important in the determination of symmetry and the departure from symmetry (Tanaka, Terauchi & Kaneyama, 1988). It is the purpose of this communication to show that the combination of symmetry elements in a number of non-centrosymmetric space groups generates loci along which, and only along which, Friedel's law holds for any thickness and for any phenomenological potential. These constitute sensitive diagnostic features for the identification of the space groups and provide a starting point for perturbative descriptions.

2. Scattering diagrams

In the multi-slice formulation of electron scattering, which is a basis-free description, a pictorial representation of the wave function can be given in terms of scattering diagrams (Moodie, 1972). Typical scattering diagrams are shown in Fig. 1.

In essence, this diagrammatic representation derives from the circumstance that the nth-order interaction can be written in the form $(i)^n \sum \ldots \sum V(g_i) \ldots V(g_{n-1}) V(g - \sum_i g_i) Z(\zeta \ldots \zeta_{n-1})$, where the $V(g_i)$ are structure amplitudes involved in the interaction and the ζ_i are the excitation errors. Each term of the series therefore consists of a function depending only on the structure multiplied by a function depending only on the geometry.

In terms of these diagrams, the breakdown of Friedel's law basically derives from the coupling of the $\pi/2$ phase change associated with each elementary scattering event within the multiple-scattering sequence with the anti-symmetric part of the structure.