

other point imperfections undoubtedly complicate the fault structure and cloud the interpretation of local fringe details.

Bovin proposes that the profuse formation of spinel-like defects may account for the degradation of sodium  $\beta''$ -alumina in operating sodium/sulfur cells. It is difficult to see how such defects can be formed when long-range oxygen-ion transport is necessary. Instead, recent experiments by De Jonghe, Feldman & Millet (1979) and Virkar & Viswanatan (1979) indicate that degradation is initiated from the sodium-ion exit electrode interface. While the formation of the blocking intergrowth due to  $\text{Na}_2\text{O}$  loss indeed produces very significant stresses, other surface flaws such as preexisting microcracks are likely to be of more significance. At present, the initiation of breakdown in sodium  $\beta$ - and  $\beta''$ -alumina is still poorly understood. Current work by Buechele, Feldman & De Jonghe (1979) seems to indicate that intrinsic degradation is not a likely cause of failure initiation. Rather, it appears that effects such as impurity deposition at the electrochemical interfaces may dominate the breakdown initiation.

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**Compensation of excess intensity in space group  $P2_1$ .** By G. D. NIGAM, *Department of Physics, Indian Institute of Technology, Kharagpur 721302, India* and A. J. C. WILSON, *Department of Physics, University of Birmingham, Birmingham B15 2TT, England*

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### Abstract

Earlier work on  $P2_1$  made simplifying assumptions. The resulting restrictions are now removed, and the expected intensity of a general reflexion is shown to be

$$\Sigma [1 - 2aJ_1(4\pi as)/(C - 4\pi a^2)s],$$

where  $\Sigma$  is the sum of the squares of the moduli of the atomic scattering factors,  $a$  is an average atomic diameter,  $J_1$  is the usual Bessel function,  $s$  is  $(2 \sin \theta)/\lambda$ , and  $C$  is the area of the face of the cell perpendicular to the twofold axis. The expected value is altered for the special groups of reflexions  $h = k = 0$  and  $l = 0$ ,  $h$  and  $k$  even.

### Introduction

Wilson (1964) showed that symmetry elements not producing systematic absences produced instead ripples in reciprocal space that modified the expected (mean) intensity of reflexion. He treated the space group  $Pm$  in some detail, and indicated how the idea of inaccessible volume could be applied to other symmetry elements, such as 2 and  $\bar{1}$ . Nigam (1972) considered the space groups  $P2_1$  and  $Pmm2$ ; his treatment of the former involved some simplifying assumptions, roughly equivalent to replacing the actual unit cell by a cylinder having the same  $c$  (twofold) axis and

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cross-sectional area equal to that of the  $C$  face. As will be seen below, this procedure is unnecessary.

Since atoms are of finite diameter, the minimum distance between a pair related by a twofold rotation axis is equal to the diameter. This will vary with the type of atom, but for the present purpose it may be assumed that all that are in contact across the axis have the same average diameter  $a$ . The  $x$  and  $y$  coordinates of the atoms, instead of being distributed with approximately uniform probability over the whole cross section of the unit cell, as assumed by Wilson (1949), are excluded from cylinders of radius  $a$  surrounding the twofold axes passing through  $00, 0\frac{1}{2}, \frac{1}{2}0, \frac{1}{2}\frac{1}{2}$ , the area available to them being thus  $C - 4\pi a^2$  instead of  $C$ . Integration over this restricted area, required in the evaluation of the expected intensity, is readily seen to be equivalent to integrating first over the whole cross section and then subtracting the integral over the interior of the excluded cylinders.

### Calculation

By the use of trigonometric identities Nigam's equation (2) can be written

$$I = \Sigma + 2 \sum_i^{\frac{1}{2}N} f_i^2 \cos 4\pi(hx_i + ky_i) + 4 \sum_{i \neq j}^{\frac{1}{2}N} \mathbf{f}_i \mathbf{f}_j^* \cos 2\pi(hx_i + ky_i) \cos 2\pi(hx_j + ky_j) \times \cos 2\pi l(z_i - z_j). \quad (1)$$

For the special case of  $h = k = 0$  this reduces to

$$I = 2\Sigma + 4 \sum_{i \neq j}^{\frac{1}{2}N} \mathbf{f}_i \mathbf{f}_j^* \cos 2\pi l(z_i - z_j), \quad (2)$$

and for  $l = 0$  to

$$I = \Sigma + 2 \sum_i^{\frac{1}{2}N} f_i^2 \cos 4\pi(hx_i + ky_i) + 4 \sum_{i \neq j}^{\frac{1}{2}N} \mathbf{f}_i \mathbf{f}_j^* \cos 2\pi(hx_i + ky_i) \cos 2\pi(hx_j + ky_j). \quad (3)$$

The average value of the first (constant) term in these equations is, of course, always  $\Sigma$  or  $2\Sigma$ , however the averaging is done. The values of the trigonometric terms require detailed consideration. In the general case of  $h, k, l$  non-zero, the integral of the trigonometric terms over the entire unit cell is zero, and the  $z$  integral in the final term is zero even in the interior of the excluded cylinders. The middle term, however, is finite within the cylinders, and it has in fact the same value for each, since  $\cos 4\pi(hx + ky)$  is unaffected by the translations  $\frac{1}{2}0$  etc. Changing to cylindrical polar coordinates gives

$$\int_0^a \int_0^{2\pi} \cos(4\pi sr \cos \varphi) r dr d\varphi = (a/2s) J_1(4\pi sa), \quad (4)$$

where  $J_s$  is the ordinary first-order Bessel function. Equation (1) then gives for the expected value of the intensity

$$E(I) = \Sigma[1 - 2aJ_1(4\pi sa)/(C - 4\pi a^2)s], \quad (5)$$

the integral having the same value for every atom. This corresponds to the first and third terms of Nigam's equation

(7), the middle one having been introduced by his method of approximation.

In the special case of  $l$  equal to zero there are additional terms arising from the double sum. Both the  $i$ th and the  $j$ th atom produce a factor like equation (4) but with  $2\pi sa$  instead of  $4\pi sa$ . Also, the translations  $0\frac{1}{2}$  etc. produce a change of sign unless  $h$  and  $k$  are even, so the contributions from the four cylinders cancel out for  $h$  or  $k$  or both odd.

For  $l = 0, h$  and  $k$  even, therefore,

$$E(I) = \Sigma[1 - 2aJ_1(4\pi sa)/(C - 4\pi a^2)s] - 16[(\Phi - 2\Sigma)a^2 J_1^2(2\pi sa)/(C - 4\pi a^2)^2 s^2], \quad (6)$$

where

$$\Phi = \left| \sum_i \mathbf{f}_i \right|^2. \quad (7)$$

For  $h$  or  $k$  or both odd, equation (5) holds even for  $l = 0$ . For  $h = k = 0$

$$E(I) = 2\Sigma \quad (8)$$

for all values of  $l$ .

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**Über den Zusammenhang zwischen der mittleren quadratischen Auslenkung  $\langle u^2 \rangle$  der Atome im Kristallgitter und der spezifischen Wärme  $c_v$  für Zink. Erratum.** Von ELISABETH ROSSMANITH, *Mineralogisch-Petrographisches Institut der Universität Hamburg, 2000 Hamburg 13, Grindelallee 48, Bundesrepublik Deutschland*

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#### Abstract

Four errors should be corrected in Rossmanith (*Acta Cryst.* (1980). A**36**, 416–420). In Fig. 1 the lowest curve (of the curves labelled 3) should be labelled  $T = 100$  K (not 300 K). In the penultimate line of the caption to Fig. 2 the reference should be to equation (6), rather than to equation (5), while in the caption to Fig. 4 the calculations for line 5 and points ● should refer to equation (5), rather than to equation (6). In

equation (5) the solidus and the letter  $m$  should be transposed:

$$\langle u^2(T) \rangle = \sum_{n=0}^{800} W(u)_{\omega_n} g(\omega_n) / m \sum_{n=0}^{800} g(\omega_n). \quad (5)$$

Die gesamte Information ist im *Abstract* enthalten.

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