

will be non-zero no matter what the value of B , and in such a situation the refinement of B or Q will not use the same modification to the scattering factors and hence the two refinements are different in this respect.

Fig. 1 shows the differences between the scattering factors modified by Q and B separately. For a particular value of Q , B is varied from 0 to 35 \AA^2 using a step of 1 \AA^2 and the values of R (vertical axis) are plotted. The summation was carried out for Bragg spacings of 10, 5, 3.3 and 2.5 \AA ; and $f(s)$ of an oxygen atom was used. The graph for $Q = 0.9$ goes through a low value around $B = 4 \text{ \AA}^2$, showing that instead of using a Q of 0.9 and a B of 0, one may use a Q of 1.0 and a B of 4 \AA^2 to obtain very similar scattering-factor curves out to 2.5 \AA . In other words, the scattering-factor curve out to 2.5 \AA obtained after refining Q to 0.9 and B to 0 is very similar to the scattering-factor curve obtained by fixing Q at 1.0 and refining B to 4 \AA^2 . However, the scattering-factor curve used after refining Q to 0.5 and B to 0 is significantly different from the scattering-factor curve used after fixing Q at 1.0 and allowing B to take any possible value.

These graphs reveal that, at medium resolution (to 2.5 \AA) for small error in Q (for example, $Q = 1.0$ is used instead of $Q = 0.9$), there exists a suitable change in the value of B (4 \AA^2) for which R is small (0.06). However, for larger errors in Q , R remains rather high for B ranging from 0 to 35 \AA^2 . Extension of the summation to smaller values of Bragg spacing obviously increases the discrepancy between

scattering factors modified independently by Q and B . These graphs show that, at medium resolution (to 2.5 \AA), B can modify scattering factors to compensate for a small error in Q , but larger error in Q cannot be accurately compensated for by B . In practice, the need to refine Q arises only for atoms suspected of disorder, and these atoms pose special problems. A disordered atom, unlike the rest of the atoms in the unit cell, may not contribute significantly to the higher-resolution diffraction patterns and hence the structure-factor least squares may tend to wipe out its contribution to higher-resolution reflections. In such situations the existence of higher-resolution data by itself may not suggest the independence of Q and B for disordered atoms. Therefore, for atoms suspected of disorder, it might be expedient to impose the desired constraints through tight restraints on B and Q rather than by elimination of variables (Hendrickson, 1985).

I thank Drs D. R. Davies, E. A. Padlan and S. Sherif for useful discussions.

References

- FREEMAN, A. J. (1962). *International Tables for X-ray Crystallography*, Vol. III, pp. 201–209. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
 HENDRICKSON, W. A. (1985). *Methods Enzymol.* **115**, 252–270.
 KUNDROT, C. E. & RICHARDS, F. M. (1987). *Acta Cryst.* **B43**, 544–547.

Acta Cryst. (1989). **A45**, 146–148

Electron microscope analyses of domains and discommensurations in ferroelectric Rb_2ZnCl_4 . Erratum.

By K. TSUDA, N. YAMAMOTO and K. YAGI, *Physics Department, Tokyo Institute of Technology, Oh-okayama, Tokyo 152, Japan*

(Received 1 November 1988)

Abstract

The following corrections should be made in Tsuda, Yamamoto & Yagi [*Acta Cryst.* (1988). **A44**, 864–870].

(1) 'only two kinds of domain boundaries' in the *Abstract* should be changed to 'two kinds of image contrast of domain boundaries'.

(2) The expressions for h_2 , h_4 , h_6 in § 4.1 should be replaced by

$$\begin{aligned} h_2: & -x \quad -y \quad -z + \frac{2}{3} \\ h_4: & -x \quad -y \quad -z \text{ (inversion)} \\ h_6: & -x \quad -y \quad -z + \frac{1}{3}. \end{aligned}$$

(3) 'two kinds of DC's showing different contrast' in the second paragraph in § 4.1 should be changed to 'two kinds of DC contrast'.

All relevant information is given in the *Abstract*.

Acta Cryst. (1989). **A45**, 146–147

International Union of Crystallography

XV International Congress of Crystallography Bordeaux, France, 19–28 July 1990 Call for programme proposals

The XV Congress of the International Union of Crystallography will be held on the Campus of Bordeaux Univer-

sity. The opening ceremony will take place on Thursday 19 July 1990 and the closing ceremony on Saturday 28 July. The Chairman of the Organizing Committee is Dr M. Hospital, Laboratoire de Cristallographie et Physique Cristalline, Université de Bordeaux I, F-33405 Talence CEDEX, France.

0108-7673/89/010146-01\$03.00

© 1989 International Union of Crystallography