

effects of polarization, absorption, or the variation of each of those quantities with deviation from the exact n -beam angle. Without detailed discussions of such quantities, the results must be accepted on faith.

It is hard to allocate blame where so many are deserving. Luckily, in this case there is enough for all.

Acta Cryst. (1975). A31, 155

Reply to Post's comments on my paper *Multiple Diffraction of X-rays and the phase problem. Computational procedures and comparison with experiment.* By R. COLELLA, *Purdue University, Physics Department, West Lafayette, Indiana 47907, U.S.A.*

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It is shown that the errors in the paper by R. Colella [*Acta Cryst.* (1974). A30, 413–423] pointed out by B. Post [*Acta Cryst.* (1975). A31, 153–155] do not in fact exist.

There is no doubt that the big difference observed between 222–113 and 222– $\bar{1}\bar{1}\bar{3}$ is due in part to the fact that the dispersion equations in the two cases involve structure factors with different magnitudes, such as $F_{11\bar{1}\bar{1}}$ and $F_{33\bar{1}\bar{1}}$, for example.

It is also true, however, that a difference between the two cases would exist *even if the structure factors were all equal*, as it happens to a good approximation in neutron diffraction. One can easily verify this statement by examining the determinantal equation [equation (8) of my paper (Colella, 1974)] and observing that the diagonal terms are essentially different in the two cases.

It is obvious that two reflections with different phases correspond to different Miller indices and therefore to different nodes in reciprocal space. The 'coupling terms' [in Post's (1975) notation] are bound to be different in any case. The intensity differences are affected by the atomic positions, besides the coupling terms. In this respect multiple diffraction can in principle solve the phase problem. The key point is that in dynamical multiple diffraction more than two beams are coherently interacting and the phases do not get lost, as it happens in two-beam diffraction without anomalous dispersion.

Ewald & Héno's (1968) treatment, quoted in the references of my paper, is essentially concerned with the Laue case and considers $2n$ solutions. As explained in my paper, the transition to the Bragg case is not a trivial one, and $4n$ solutions must be considered when some of the diffracted beams are parallel to the surface of the crystal. Substantial changes are involved in the boundary conditions.

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Schottky defects in KI and RbI. By P. D. PATHAK and N. M. PANDYA, *Physics Department, Gujarat University, Ahmedabad, India*

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The temperature dependence of the thermal expansion of KI and RbI at high temperatures is shown to be related to the concentration of thermally generated Schottky defects. The experimental value of the energy of formation of these defects for RbI has been estimated for the first time. The two halides are found to obey the 'law of corresponding states' established by Pathak & Vasavada [*Acta Cryst.* (1970). A26, 655–658].

Introduction

The experimental value of the energy of Schottky-pair formation for KI has been determined by Ecklin, Nadler &

References

- COLE, H., CHAMBERS, F. W. & DUNN, H. M. (1962). *Acta Cryst.* **15**, 138–144.
 COLELLA, R. (1974). *Acta Cryst.* **A30**, 413–423.
 EWALD, P. P. & HÉNO, Y. (1968). *Acta Cryst.* **A24**, 5–15.

My failure to observe Umweganregung effects on the 400 with Co $K\alpha$ was in fact due to a large vertical divergence (of the order of 1°). Since these are the conditions in which most of the crystallographic work is done, I felt that it would be of some interest to develop a procedure for predicting whether not Umweganregung effects might be present in given experimental conditions.

As to my statement concerning the ratio (or ratios?) between Umweganregung peaks, it is neither trivial nor incorrect. It is only limited to one particular experiment and its main value is to stimulate further research in this area. That the Umweganregung peaks generally increase upon grinding is a rather obvious result and had been previously reported (Colella & Merlini, 1966).

I do not understand the statement about the different angles formed by the (113) and ($\bar{1}\bar{1}\bar{3}$) planes with (222) in relation to the effects produced by grinding, and I believe that it is not justified.

The other points of Post's paper seem to me irrelevant or inconsequential.

References

- COLELLA, R. (1974). **A30**, 413–423.
 COLELLA, R. & MERLINI, A. (1966). *Phys. Stat. Sol.* **18**, 157–166.
 EWALD, P. P. & HÉNO, Y. (1968). *Acta Cryst.* **A24**, 5–15.
 POST, B. (1975). **A31**, 153–155.

Rossel (1964). A similar value for RbI is not available in the literature. Theoretical attempts to estimate these values have been made by Boswarva & Lidiard (1967), Rao & Rao (1968) and others.