SHORT COMMUNICATIONS

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Acta Cryst. (1980). A**36**, 827

Comment on *The number of permitted modes of propagation in N-beam dynamical diffraction of X-rays* by S. L. Chang.

By Roberto Colella, *Purdue University, Physics Department, West Lafayette, Indiana* 47907, *USA*

(*Received* 29 *November* 1979; *accepted* 12 *February* 1980)

Abstract

Attention is directed to a previous treatment of multi-beam diffraction of X-rays by Colella [*Acta Cryst.* (1974), A**30**, 413–423]. The rules governing the number of permitted modes are discussed and compared with those given in a recent article by Chang [*Acta Cryst.* (1979), A**35**, 543–547].

Chang (1979) fails to recognize that the problem of N-beam dynamical diffraction for X-rays (Bragg case) has been previously investigated, for the first time, and solved in the most general situation by the present author (Colella, 1974). The rule governing the number of beams existing in the crystal is discussed in great detail and derived in § 3 of my paper, in which no approximations are introduced relative to the asymmetry of the reflections involved, namely to the magnitude of the angles between incident (and diffracted) beams and the surface of the crystal. It is shown in my paper that, under any circumstances, the number of beams actually excited in the crystal N_p is fixed: $N_p = 2N$, irrespective of the magnitude of the excitation error (for a thick crystal).

It will be recalled here that two three-beam cases were studied in detail in my 1974 paper, the integrated intensities of the 222–113 and 222–$\bar{1}\bar{1}3$ *Umweganregung* peaks in germanium, and compared with experimental results. The agreement between theory and experiment was within 5%, which can be considered excellent, in view of the experimental and computational difficulties involved.

Since the rule derived by Chang is different [$N_p = 2(N - N_{\rm Bragg})$], I believe that a comment is in order. In Chang's treatment the case of grazing beams (incident and diffracted) is avoided. In such a case it is legitimate to linearize the dispersion equations, and the total number of beams excited in the crystal is $2N$, in general, instead of $4N$, as described in my paper. Since in Chang's treatment it is legitimate to distinguish between Bragg and Laue beams, it is possible to neglect the Bragg beams in computing N_p, because Bragg beams can only exist in a crystal if reflected by the exit surface. Such beams correspond to waves of *increasing amplitudes*, and do not exist in absorbing crystals of infinite thickness. The rule $N_p = 2(N - N_{\rm Bragg})$ follows, therefore, from this consideration.

The same argument involving waves of increasing amplitudes has made it possible, in my treatment, to reduce the number of excited beams from $4N$ to $2N$. Since the dispersion equations have not been linearized in my treatment, in order to consider the case of grazing beams, it is to be expected that a larger number of beams may result, some of which are of negligible intensity when there are no grazing beams.

It is concluded, therefore, that there is no contradiction between the rules governing the number of excited beams in Chang's paper and mine.

May I also point out that the same rule, $N_p = 2N$, has been obtained in an independent treatment of N-beam diffraction in the Bragg case which has just appeared in the literature (Kohn, 1979).

0567-7394/80/050827-01$01.00

References

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Kohn, V. G. (1979). *Phys. Status Solidi A*, **54**, 375–384. See p. 378.