[23] A. Sommerfeld, Atombau und Spektrallinien, Verlag Vieweg, Braunschweig 1939, Band 1.
Hierbei zeigte sich, daß Gl. (15) auf S. 303 in [23], die zur Berechnung der Abschirmkonstante 3s,p dient, einen falschen Zahlenfaktor enthält. Die Gleichung muß richtig lauten:

$$(Z-s)^2 = \left(\frac{3}{\alpha}\sqrt{\frac{6\,\Delta\nu}{R}} - \frac{279}{16}\,\frac{\Delta\nu}{R}\right)\left(1 + \frac{2807}{1024}\,\alpha^2\,\frac{\Delta\nu}{R}\right).$$

[24] J. A. Bearden, Rev. Mod. Phys. **39,** 78 [1967].
[25] E. Persson u. O. E. Efimov, Phys. Stat. Sol. **(a) 2,** 757 [1970].
[26] D. Ling u. H. Wagenfeld, Phys. Lett. **15,** 8 [1965].
[27] B. W. Batterman, Phys. Rev. **133,** A 759 [1964].
[28] B. W. Batterman, Phys. Rev. **126,** 1461 [1962].
[29] J. J. MeMarco u. R. J. Weiss, Phys. Rev. **137,** A 1869 [1965].
[30] U. Bonse, Z. Physik **161,** 310 [1961].
[31] B. Okkerse, Phil. Res. Rep. **17,** 464 [1962].
[32] E. W. Pike, J. Appl. Phys. **12,** 206 [1941].
[33] M. Lefeld-Sosnowska, Phys. Stat. Sol. **7,** 449 [1964].
[34] R. B. Roof, Phys. Rev. **113,** 826 [1959].
[35] A. Authier, Acta Cryst. **14,** 287 [1961].
[36] International Tables for X-Ray Crystallography, Vol. III, Birmingham 1962.
[37] J. Ludewig, Acta Cryst. **A 25,** 116 [1969].
[38] J. Ludewig, Z. Naturforsch. **28 a** [1973], Heft 7.
[39] N. Kato, J. Phys. Soc. Japan **10,** 46 [1955].
[40] L. P. Hunter, J. Appl. Phys. **30,** 874 [1959].
[41] S. Maruyama u. G. Honjo, J. Phys. Soc. Japan **17,** 1803 [1962].
[42] O. N. Efimov u. E. K. Kovev, Phys. Stat. Sol. **17,** 397 [1966].
[43] B. W. Batterman u. D. R. Chipman, Phys. Rev. **127,** 690 [1962].
[44] C. Ghezzi, A. Merlini u. S. Pace, Nuovo Cim. **49,** 58 [1967].
[45] R. N. Kyutt u. O. N. Efimov, Sov. Phys. – Sol. State **11,** 228 [1969].
[46] Y. H. Ohtsuki u. S. Yanagawa, J. Phys. Soc. Japan **21,** 502 [1966].
[47] A. M. Afanasev u. Yu. Kagan, Acta Cryst. **A 24,** 163 [1968]; A. M. Afanasev, Yu. Kagan u. F. N. Chukhovskii, Phys. Stat. Sol. **28,** 287 [1968].
[48] H. Sano, K. Ohtaka u. Y.-H. Ohtsuki, J. Phys. Soc. Japan **27,** 1254 [1969].
[49] P. H. Dederichs, mündliche Mitteilung.
[50] O. N. Efimov, Phys. Stat. Sol. **22,** 297 [1967].
[51] C. Ghezzi, A. Merlini u. S. Pace, Phys. Rev. **B 4,** 1833 [1971].
[52] G. Hildebrandt, Veröffentlichungen der Herbstschule über Grundlagen und Anwendungen der dynamischen Interferenztheorie, Stolberg (DDR), 1972.

6-Beam Borrmann Diffraction †

T. C. Huang *, M. H. Tillinger, and Ben Post

Physics Department, Polytechnic Institute of Brooklyn, Brooklyn, N.Y.

(Z. Naturforsch. **28 a,** 600—603 [1973]; received 1 February 1973)

Dedicated to Professor Dr. G. Borrmann on his 65th birthday

Linear absorption coefficients and transmitted intensities have been calculated for all twelve modes of propagation in one case of 6-beam diffraction of x-rays through germanium. At the 6-beam point the absorption coefficients of four of the modes are less than 1 cm^{-1}, using CuKα_1 radiation, compared with the "normal" value of 352 cm^{-1}; one third of the energy incident on the crystal at the exact 6-beam angle is allocated to these low absorption modes.

Introduction

The observation by Borrmann and Hartwig [1] that the intensity of the (111) reflection, anomalously transmitted through germanium crystals, is enhanced further when $(11\bar{1})$ is also in diffraction position, has renewed interest in simultaneous diffraction effects in perfect crystals. Several theoretical investigations of these effects have since been reported [2]; the work of Joko and Fukuhara [2] is especially noteworthy. They investigated several cases of 3-beam, 4-beam and 6-beam multiple diffraction and calculated numerical values of the lowest absorption coefficients for the exact n-beam point in each case.

Their 6-beam results are of particular interest. The geometry of this case of simultaneous diffraction is illustrated in Figure 1. The six reciprocal lattice points lie in a plane perpendicular to [111] at the vertices of a regular hexagon. All six will diffract simultaneously if the crystal is rotated about $[\bar{2}11]$ until $(0\bar{4}4)$ is brought to diffracting position. Joko and Fukuhara's calculations indicated that the absorption coefficient of one of the twelve modes of propagation vanishes when 6-beam diffraction oc-

† Supported in part by the Office of Naval Research under Contract No. N00014-67-A-0438-005.

* Present address: IBM, Systems Product Division, Essex Junction, Vt. 05452.

Reprint requests to Professor B. Post, Physics Department, Polytechnic Institute of Brooklyn, 333 Jay Street, *Brooklyn, N. Y. 11201,* U.S.A.

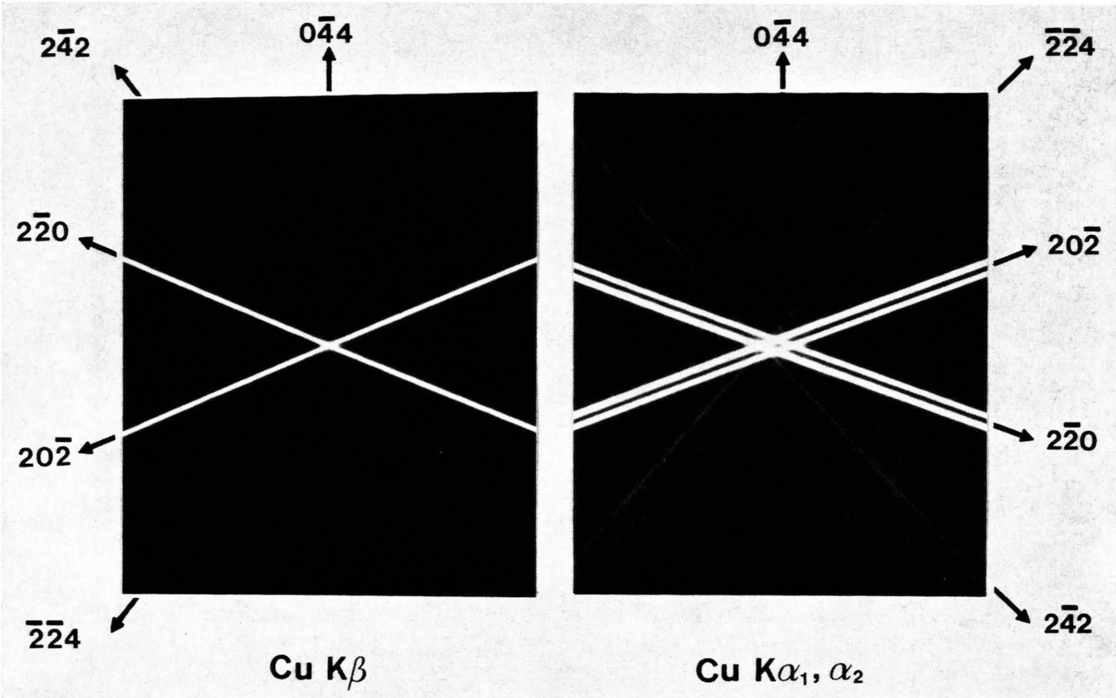

Fig. 3. 6-beam case: Forward diffracted beams (t=0.5 mm).

curs. The authors did recognize that errors in the published values of the imaginary parts of the atomic scattering factors could lead to minor inaccuracies in their results and that the lowest absorption coefficient was probably slightly greater than zero. It was clear, nevertheless, that a remarkable reduction in at least one of the absorption coefficients occurs in the 6-beam case.

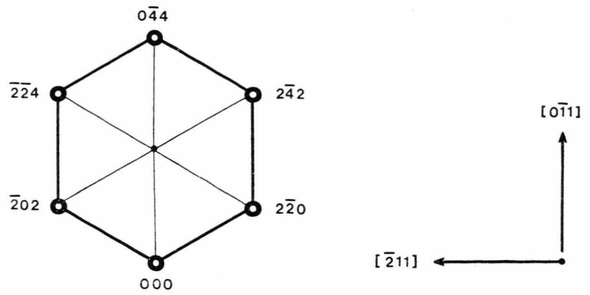

Fig. 1. Geometry of the six-beam case.

We have extended the Joko and Fukuhara 6-beam calculations to include values of the excitations absorption coefficients and transmitted intensities of all 6-beams for the twelve modes of propagation over a wide range of incident beam settings about the exact 6-beam point. We have also begun an experimental study and present some preliminary findings.

Experimental

The experimental setup used in our work is illustrated schematically in Figure 2. An unfiltered incident microbeam ($100 \times 100\ \mu$) from a copper target was used in conjunction with a large specimen-to-film distance. The relatively large divergence of the incident beam (6°) facilitated alignment of the crystal and the large specimen-to-film distance yielded satisfactory resolution [3].

Photographs of the forward diffracted beams were obtained using a 0.5 mm thick germanium crystal with Cu$K\alpha_1$, α_2 and β radiations and are shown in Figure 3 *. The very intense 2-beam lines are due to reflections of the form $\{220\}$; the two of moderate intensity are due to $\{422\}$ and the very weak reflection is the $(0\bar{4}4)$. The enhancement expected at the 6-beam point was not observed on either photograph. Our subsequent calculations indicated that substantially thicker crystals would be needed to display clearly the 6-beam enhancement relative to the (220) lines. Such thick, relatively perfect crystals were not available to us when these photographs were obtained but will be investigated in the near future.

Calculations

For the calculation of multiple beam dynamical effects we prepared computer programs ** based on the plane wave dynamical theory of Ewald [4], as modified by von Laue [5].

In Table 1 we list values of the linear absorption coefficients and the corresponding excitations for each of the twelve modes of propagation calculated for the exact n-beam point. The absorption coefficient for mode 1 is .02 cm^{-1}, in good agreement with the corresponding value calculated by Joko and

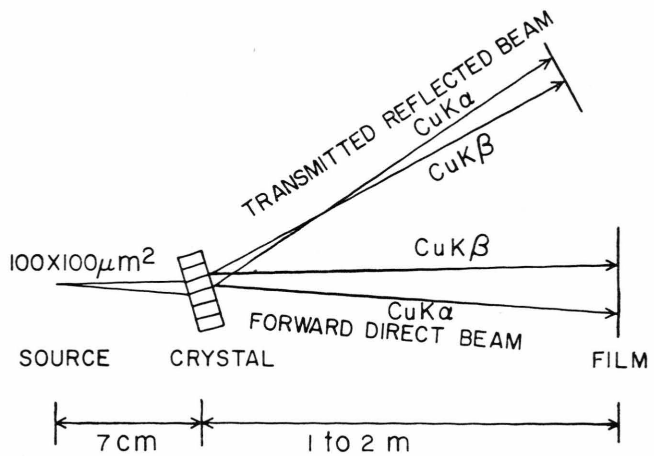

Fig. 2. Schematic diagram of experimental arrangement.

* Figure 3 see page 600 a.

** Details of the computing methods will be included in a manuscript, now in preparation, dealing with various 3- and 4-beam cases.

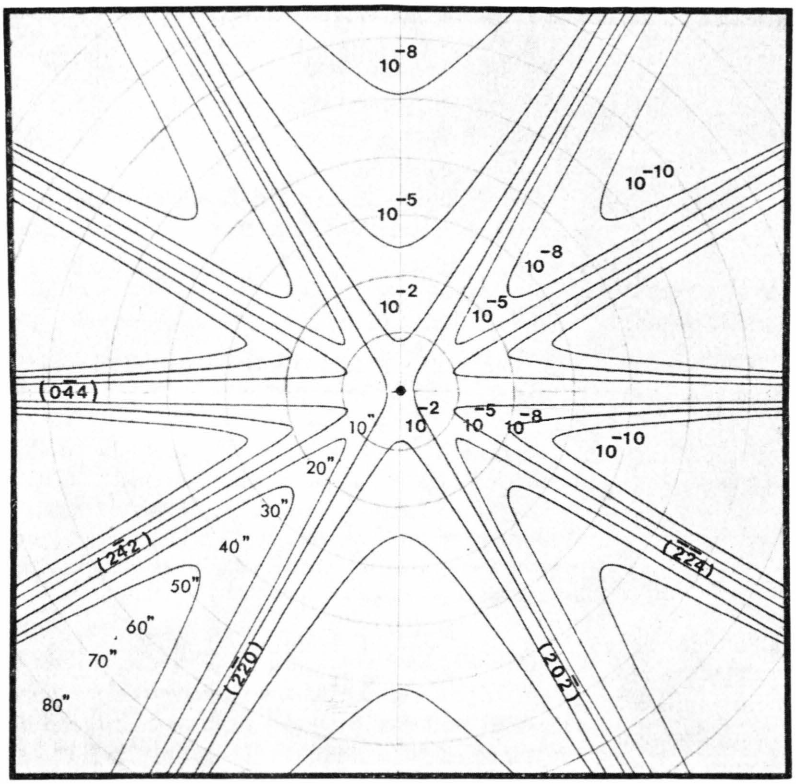

Fig. 4. I_{000} vs. $\Delta\Theta$ (t=0.5 mm).

Fukuhara. We note also that fully one-third of the incident energy is allocated to modes having absorption coefficients significantly less than 1 cm^{-1}.

Table 1. μ's and excitations at the exact 6-beam pt. for CuKα_1 radiation.

Mode	μ cm^{-1}	Excitation	
1	0.02	1/12	1/3
2	0.16	1/18	
3	0.16	1/9	
4	0.48	1/12	
5	38.72	1/18	1/3
6	38.72	1/9	
7	60.02	1/18	
8	60.02	1/9	
9	85.43	1/12	1/3
10	1,186.16	1/12	
11	1,377.79	1/18	
12	1,377.79	1/9	
	μ_{ave} = 352.12		

Values of $I_{000}/I_{inc.}$ transmitted through a 0.5 mm thick crystal are plotted in Fig. 4 as a function of $\Delta\Theta$ (deviation from the exact 6-beam angle). It is clear that, for this thickness, observation of the enhanced 6-beam point would be difficult, particularly when the divergences of the various beams are taken into account. Calculations, similar to that of Fig. 4, for much thicker crystals indicate very low values of transmitted intensities except for the 6-beam point.

A map of the mode 1 wavefield in the germanium crystal, projected along [111] brings out more clearly the physical basis of the anomalously low 6-beam absorption (Figure 5). The average position of each germanium atom is at a node of the electric field in the 6-beam case. A similar statement may be made for the (220) case, and for all others where $h+k+l=4n$. One significant difference is brought out clearly by Fig. 6, a plot of the wavefield due to the minimum absorption modes for both the 6-beam case and for (220), along a line parallel to [2$\bar{1}\bar{1}$] passing through three atomic centers. It is evident that in the (220) case, thermal atomic vibrations at room temperature must bring the atoms into regions where the electric field differs significantly from zero. This effect, which was investigated by Ludewig [6] is primarily responsible for the residual minimum absorption coefficient of 15.3 cm^{-1} in the (220) case. In the much larger nodal regions in the 6-beam cases, atomic vibrations at room temperature do not have this effect and the absorption therefore remains close to zero.

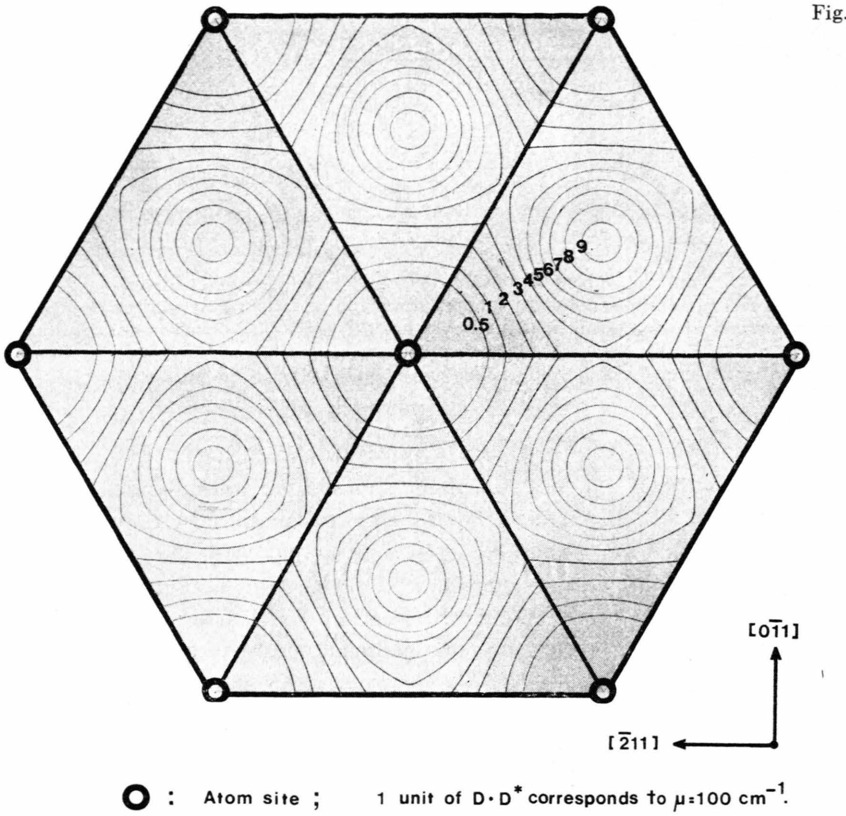

Fig. 5. Projection of $D \cdot D^*$ onto (111), [mode 1].

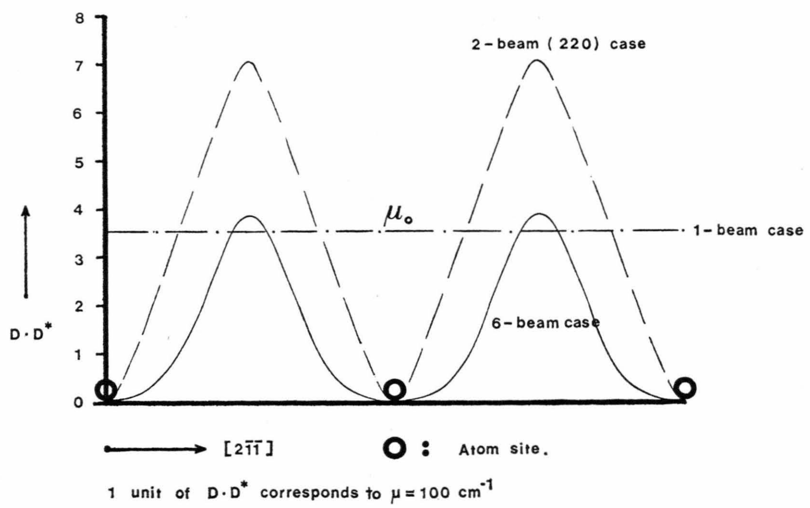

Fig. 6. $D \cdot D^*$ along [2$\bar{1}\bar{1}$], (mode 1).

[1] G. Borrmann and W. Hartwig, Z. Kristallog. **121**, 401 [1965].

[2] a) T. Joko and J. Fukuhara, J. Phys. Soc. Japan **22**, 597 [1967]; b) P. Penning and D. Polder, Philips Res. Rep. **23**, 1 [1968]; c) P. P. Ewald and Y. Heno, Acta Cryst. **A 24**, 1 [1968].

[3] R. Feldman and B. Post, Phys. Stat. Sol. (a) **12**, 273 [1972].

[4] P. P. Ewald, Ann. Phys. (Leipzig) **49**, 117 [1916].

[5] M. v. Laue, Röntgenstrahl-Interferenzen, Akademischer Verlag, Frankfurt 1960.

[6] J. Ludewig, Acta Cryst. **A 25**, 116 [1969].