

developed by Campos, Cardoso and Caticha-Ellis (1983), J. Appl. Cryst. 16, 360. It must be noticed that the F's obtained by this method are automatically corrected for absorption, L.P. and extinction. A further improvement which facilitates the calculation by decreasing  $n$ , consist in using as a rotation axis a crystallographic direction which does not coincide with any symmetry axis and corresponds to a forbidden reflexion. The effect is striking: 4 or higher order beam interactions are decoupled in 3-beam cases thus simplifying the calculations; secondary equivalent reflexions (which would lead to Bijvoet pairs in anomalous dispersion are clearly distinguished without the use of specially chosen wavelengths. "Absolute" indexing i.e. indexing with respect to the chosen axes is immediately possible. The results applies independently of the presence of a center of symmetry in the structure. As examples the cases of rutile and silicon cut in the direction (201) will be shown.

reflections. The experimental method used in our measurements involves very low intensities even when using a rotating anode generator. However it seems very promising in the determination of bonding electron distribution in covalent structures. The use of synchrotron radiation is envisaged for further, more precise measurements. Some preliminary results will be given.

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11.8-4 STRUCTURE FACTORS OF SOME "FORBIDDEN" REFLECTIONS OF SILICON CRYSTALS OBTAINED BY MULTIPLE DIFFRACTION OF X-RAYS. By S. Caticha-Ellis and Lisandro P. Cardoso. Instituto de Física - UNICAMP - C.P. 6165, 13100, Campinas, SP, BRAZIL.

The space group forbidden reflection 222 of diamond-type structures, first detected by Sir W.H. Bragg in 1921, has been the subjected of many investigations and were measured for diamond, Si and Ge by many authors (for ex. Penninger (1937,60), Weiss (1964,66), Colella & Merlini (1966), Kohra and collab. (1971,74)). The importance of the measurements is of course the determination of the anti-symmetric part of the electron density, i.e., that of bonding electrons, whose geometry does not conform with atomic spherical scattering factors. Different experimental methods had been used, such as reflection profile, pendellösung fringes, integrated intensity with parallel and divergent beam, etc. Almost all the authors state that they tried to avoid measuring under conditions of multiple diffraction. Actual measurements of other forbidden reflections with  $h+k+l=4n+2$ , have been so far reported as negative; reflection 420 seems to have been observed by Wittels (1966) in doped Ge crystals but Colella & Merlini state that they could not observe it and conclude that it should be at least 20 times smaller than 222. Renninger was able to give upper limits for the 442 and 622.

By using the decoupled multiple diffraction method (Cardoso and Caticha-Ellis this meeting) with forbidden primary reflection of the type  $4n+2$  without symmetry it is possible in principle to measure several other "forbidden"

11.8-5 EXPERIMENTAL TEST OF Kawamura and Kato's SECONDARY EXTINCTION CORRECTION FORMULA By J. Harada, H. Miyatake and M. Sakata, Faculty of Engineering, Nagoya University, Chikusa-ku, Nagoya, Japan.

Recently, Kawamura and Kato (Acta Cryst. (1983) A39, 305) presented an analytical formula for extinction and absorption corrections to the integrated Bragg intensity data collected from a spherical or cylindrical single crystal on the basis of Kato's new statistical dynamical diffraction theory. Though they have made a theoretical comparison with the widely accepted Becker and Coppens formula, any experimental test of the two theories so far seems to have not reported yet. Hence it is still not well understood the difference of the results when applying the two theories, particularly from the practical view point. We have carried out such a comparison with the use of the data sets collected by both angle and energy dispersive neutron diffraction methods. It is revealed that both theories gave the same answer for the data by the conventional angle dispersive method, even though some reflections are noticed to be severely affected by extinction effect, while they gave a slightly different parameter sets for the data by energy dispersive method.