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AN ALGORITHM FOR CALCULATING THE BRAGG ANGLES AND INTERPLANAR SPACINGS FOR DIFFRACTION MAXIMA COMPATIBLE WITH THE SPACE GROUP REQUIREMENTS

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A program, DTHETA, is written in FORTRAN 5 for UNIVAC 1100, which calculates the Bragg angles, Θ, and the interplanar spacings, d, for diffraction maxima compatible with the space group requirements. The output results (a table containing the Miller indices hkl, d, d^{-2}, Θ, $\sin\Theta$, $\sin^2\Theta$, together with the crystal and reciprocal unit cell parameters) are printed out in order of increasing Θ values. For a group of two or more mutually equal Bragg angles, corresponding to various combinations of Miller indices, which are symmetrically equivalent, only one combination of the indices is printed out. The listing of the program is available from the authors.

In investigation of solids by X-ray and neutron diffraction it is useful to have a program which calculates the Bragg angles, Θ_{hkl}, of the theoretically possible diffraction maxima (i. e. reflexions) in accordance with the space group requirements. The Bragg angles, characterizing a given crystalline substance, are measured in diffraction experiment. The Bragg angle of a diffraction maximum is given by the well-known equation,

$$\lambda = 2d_{hkl} \sin \Theta_{hkl}, \qquad (1)$$

where λ is the wavelength of the radiation used to obtain the diffraction pattern, and d_{hkl} is the interplanar spacing for the corresponding set of crystal lattice planes with the Miller indices *hkl*. The interplanar spacings can be calculated, in a general triclinic case, according to the formula

$$d_{hkl}^{-2} = h^2b_1^2 + k^2b_2^2 + l^2b_3^2 + 2hkb_1b_2\cos\beta_3 + 2klb_2b_3\cos\beta_1 + 2lhb_3b_1\cos\beta_2, \quad (2)$$

where b_i and β_i (i = 1, 2, 3) are the unit cell parameters of the reciprocal lattice. These are defined through the unit cell parameters of the crystal lattice, a_i and α_i (i = 1, 2, 3), as follows[1]:

$$b_i = (a_i \sin\alpha_{i+1} \sin\beta_{i+2})^{-1},$$

$$\cos\beta_i = \frac{\cos\alpha_{i+1}\cos\alpha_{i+2} - \cos\alpha_i}{\sin\alpha_{i+1}\sin\alpha_{i+2}},$$

with $\alpha_{i+3} = \alpha_i$, $\beta_{i+3} = \beta_i$.

The interplanar spacings are to be calculated from (2) only for those *hkl* which are permissible for a given space group. Then the corresponding Bragg angles are obtained from (1).

If the space group is not known, but some of the symmetry elements are determined or may be forseen, then the d_{hkl}'s and Θ_{hkl}'s of only those reflexions, which are required for the supposed symmetry elements, can be calculated. Also, if the unit cell parameters of the crystal lattice are not accurately known, the calculation of the possible d_{hkl}'s and Θ_{hkl}'s may be of much help.

For a group of two or more mutually equal Bragg angles, corresponding to various combinations of Miller indices, which are symmetrically equivalent, it is desirable to list only one combination of the indices. For cubic crystals the Miller indices are permutable, and it is the same with the indices *h* and *k* in tetragonal and hexagonal systems. All such permutations are symmetrically equivalent. As further examples, the Miller indices *hk*0 and $\bar{h}k0$ in monoclinic, and the indices *hkl* and $\bar{h}\bar{k}\bar{l}$ in triclinic system, are also symmetrically equivalent.

Finally, it is very desirable that the Bragg angles, compatible with the above requirements, are listed in order of increasing values. Then the lists of the calculated and observed Bragg angles are directly comparable, this yiedling the Miller indices of each observed reflexion.

All the above points are taken into account in a program, DTHETA, written recently in FORTRAN 5 (for UNIVAC 1100) by the authors. The input data for the program are as follows:

1st card: Title, including name, compound, space group, possible reflexions, date etc.

2nd card: Unit cell parameters, a_i and α_i.

3rd card: X-ray wavelength, λ; the smallest value of the interplanar spacing up to which the calculation is to be carried out, d_{min}.

4th card: Minimum and maximum values of Miller indices, i. e. the ranges of the Miller indices within which the calculation is to be carried out.

5th card: Index (integer) denoting the crystal system, INDCRS; index (integer) denoting the lattice type, LATTCE; number of classes of special reflexions with general conditions for possible reflexions, NSPREF. If NSPREF = 0 the 5th card is the last input card.

6th card: This card contains NSPREF indexes (integers) denoting particular classes of special reflexions, ISPREF. For instance, ISPREF = 1, 2, 3, 4,... for the classes of special reflexions $0kl$, $h0l$, $hk0$, hhl,... resp.

7th card: This card contains NSPREF indexes (integers) denoting conditions for possible special reflexions, IPOREF. For instance, if ISPREF = 1, IPOREF = 1, 2, 3, 4 for the conditions $k = 2n$, $l = 2n$, $k + l = 2n$, $k + l = 4n$, resp.

As output, the program gives the input data, the unit cell parameters of the reciprocal lattice, b_i and β_i ($i = 1, 2, 3$), and a table with values of hkl, d_{hkl}, d_{hkl}^{-2}, Θ_{hkl}, $\sin\Theta_{hkl}$ and $\sin^2\Theta_{hkl}$.

The program has been tested for a series of substances belonging to various space groups and all crystal systems. The average total computing time is 1-2s, CAU time is 0.2—0.5s, and the average memory is 8K. The listing of the program is available on request.

During the testing of our program a note by Arzi[2] appeared in J. appl. Cryst. entitled »A program to generate Bragg reflexions compatible with lattice type and systematic absences«. Arzi's program is based on a quite different scheme than ours. Namely, the reflexions compatible with the space group are taken into account choosing as input data integers U, V, W, Z, Y satisfying the formulae for systematic absences in the form

$$Uh + Vk + Wl = Zn - Y,$$

n being an integer incremented by the program. It is not stated whether the program includes the elimination of symmetrically equivalent reflexions.

References

1) *International Tables for X-ray Crystallography,* Vol. 2, p. 106, The Kynoch Press, Birmingham, 1967;

2) E. ARZI, J. appl. Cryst. **13**, 100 (1980).

ALGORITAM ZA RAČUNANJE BRRAGOVIH KUTOVA I MEĐUMREŽNIH RAZMAKA ZA DIFRAKCIJSKE MAKSIMUME U SKLADU SA ZAHTJEVIMA PROSTORNE GRUPE

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Napisan je program, DTHETA, u FORTRAN-u 5 za UNIVAC 1100, koji računa Braggove kutove, Θ, i međumrežne razmake, d, za difrakcijske maksimume u skladu sa zahtjevima prostorne grupe. Izlazni rezultati (tablica koja sadrži Millerove indekse hkl, d, d^{-2}, Θ, $\sin\Theta$, $\sin^2\Theta$, zajedno s parametrima kristalne i recipročne jedinične ćelije) štampaju se u nizu rastućih vrijednosti Θ. Za grupu od dva ili više međusobno jednakih Braggovih kutova, koji odgovaraju raznim, ali simetrijski ekvivalentnim, kombinacijama Millerovih indeksa, štampa se samo jedna kombinacija Millerovih indeksa. Tekst programa može se dobiti od autora.

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