estimate' for T was obtained by substituting Zachariasen's approximation for D in (5).

The diffracted- and transmitted-beam rocking curves presented in Figs. 1 and 2 show that the present expressions based on (2) lead to much smoother behaviour than those based on Zachariasen's approximation for D. Furthermore, the expected complementary behaviour of T and R is exhibited by the present results but is not exhibited by those based on Zachariasen's approximation.

It may be noted that Zachariasen's approximation is valid for all the cases illustrated in his book, but it is not necessarily valid for *all* cases, whereas (2) will always be correct within the framework of Zachariasen's explicit assumptions. Moreover, there does not appear to be any good reason for making Zachariasen's approximation, since D given by (2) is just as easy to evaluate as D in Zachariasen's approximation.

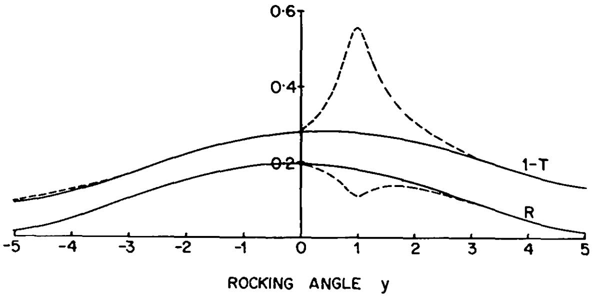

Fig. 1. Reflectivity (R) and transmissivity (T) rocking curves for a centrosymmetric crystal in the *symmetric* Bragg case ($\beta = 0$) plotted against the rocking angle y [defined in equation (3.181) of Zachariasen] for $A = 0{\cdot}5$, $g = -0{\cdot}1$ and $\kappa = +0{\cdot}1$. The solid curves are the solutions given by equations (1) and (2), while the broken curves were obtained by taking Zachariasen's approximation for D.

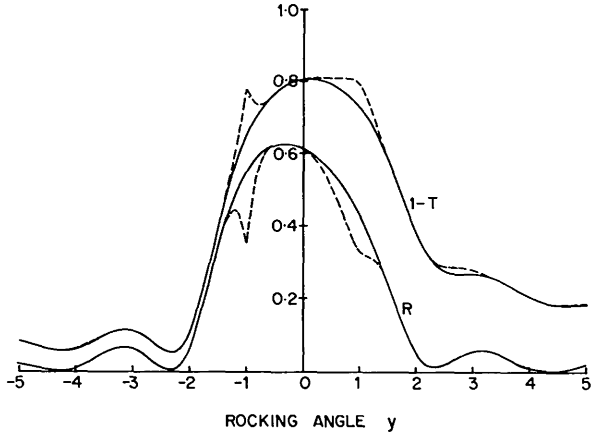

Fig. 2. As for Fig. 1 but with equations evaluated for *asymmetric* Bragg case ($\beta = +0{\cdot}8$) and $A = 1{\cdot}5$, $g(0) = -0{\cdot}1$ [$g(\beta) = g(0)/(1-\beta^2)^{1/2}$] and $\kappa = +0{\cdot}1$.

In conclusion, we note that the precise form of thin-crystal rocking curves is currently of practical interest. For example, Kohra (1972) and his group have measured (virtually intrinsic) thin-crystal rocking curves for Si.

References

Fingerland, A. (1971). *Acta Cryst.* A**27**, 280–284.

Kohra, K. (1972). *Proc. Int. Conf. on X-Ray and Optical Microanalysis*, pp. 35–45. Tokyo: Tokyo Press.

Zachariasen, W. H. (1945). *Theory of X-Ray Diffraction in Crystals*, Chap. 3. New York: John Wiley.

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On extrinsic faults in face-centred cubic crystals.

By Hidewo Takahashi, *Faculty of Education, Kagoshima University, Kagoshima, Japan*

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Application of the matrix intensity equation of X-ray diffraction is discussed for the second problem of extrinsic faults in face-centred cubic crystals, discussed by Howard [*Acta Cryst.* (1977), A**33**, 29–32]. The second problem is generalized to the case that the probability with which inserted layers follow layers of the original crystal differs from that with which inserted layers follow previously inserted layers. The **Q** matrix for the case is obtained and the results of intensity calculation are shown.

Recently, Howard (1977) solved the second problem of extrinsic faults in face-centred cubic crystals by the use of the difference equation. We can obtain the same results by application of the matrix intensity equation of X-ray diffraction. Application of the matrix intensity equation to growth, growth and deformation, and multiple-deformation faults in various close-packed structures was discussed by the present author (Takahashi, 1976). Extrinsic faults in f.c.c. crystals are equivalent to double-deformation faults. Our **Q** matrix is different from that of Kakinoki & Komura (1965). As is well known, the **P** matrix is a transition probability matrix of the Markov process. The original definition of the **P** matrix by Kakinoki & Komura (1965) is that the ij element of the **P** matrix is the probability of finding the layer j after the layer i. That is to say, states are defined by kinds of layers in their treatment. States and transition probabilities are called complexions and continuing probabilities, respectively, in this article. Complexions can be defined by sequences of layers or displacement vectors in the matrix intensity equation. If the ith complexion is followed by the *j*th complexion, the vector directed from the origin of the last layer of the *i*th complexion to that of the *j*th is denoted by $\mathbf{t}_j = \mathbf{d}_j + \mathbf{c}_j$, where $\mathbf{d}_j$ is the parallel component and $\mathbf{c}_j$ is the normal component to the layer planes, and the *j*th element of our diagonal matrix $\mathbf{\Phi}$ becomes $\varepsilon_j = \exp\{-2\pi i[(\mathbf{s} - \mathbf{s}_0)/\lambda]\,\mathbf{t}_j\}$. We can choose the origin of the layers in order that the *j*th element ε_j does not depend on any preceding complexion. Then, our $\mathbf{Q}$ matrix is expressed by $\mathbf{P\Phi}$, that is, the *j*th column of the $\mathbf{Q}$ matrix is the *j*th column of the $\mathbf{P}$ matrix multiplied by ε_j. The diffracted intensity can be calculated if we know the coefficients of the characteristic equation of the $\mathbf{Q}$ matrix by the method described by Kakinoki & Komura (1965). From a practical point of view, it is not necessary to derive the characteristic equation of the $\mathbf{Q}$ matrix, since we can calculate the coefficients from the $\mathbf{Q}$ matrix by Newton's formula on an electronic computer.

For multiple-deformation faults, complexions are defined by the displacement vectors, $\mathbf{d}_1 = \frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}$ and $\mathbf{d}_2 = \frac{1}{3}\mathbf{a} + \frac{2}{3}\mathbf{b}$, the positions of the displacement vectors in the sequence of the displacement vectors which indicates the sequence of layers in fault-free structures, and the values of continuing probabilities P_{ij}. Since the vector sequence of f.c.c. crystals is $\mathbf{d}_1\mathbf{d}_1\mathbf{d}_1 \ldots$ or $\mathbf{d}_2\mathbf{d}_2\mathbf{d}_2 \ldots$, any position is equivalent to any other, so that the complexions are distinguished by the displacement vectors and by the continuing probabilities. We denote complexions which follow preceding ones with probability $(1-p)$ by $\mathbf{d}_1$ and $\mathbf{d}_2$ and those which follow preceding ones with probability p by $\mathbf{d}'_1$ and $\mathbf{d}'_2$, where the probability that any layer is followed by an inserted layer is denoted by p. We obtain the following sequences of the complexions from Fig. 1 of Howard (1977). Complexion $\mathbf{d}_1$ is followed by $\mathbf{d}_1$ and $\mathbf{d}'_2$, $\mathbf{d}'_2$ is followed by $\mathbf{d}_2$ and $\mathbf{d}'_1$, $\mathbf{d}_2$ is followed by $\mathbf{d}_1$ and $\mathbf{d}'_2$, and $\mathbf{d}'_1$ is followed by $\mathbf{d}_1$ and $\mathbf{d}'_2$. When we number the complexions as follows,

$$\mathbf{d}_1 = 1, \quad \mathbf{d}_1 = 2, \quad \mathbf{d}'_1 = 3, \quad \mathbf{d}'_2 = 4, \tag{1}$$

the elements of the $\mathbf{P}$ matrix become

$$\begin{aligned} &P_{11} = P_{21} = P_{31} = P_{42} = (1-p), \\ &P_{14} = P_{24} = P_{34} = P_{43} = p, \end{aligned} \tag{2}$$

and the other elements are zero. Hence, the elements of the $\mathbf{Q}$ matrix are:

$$\begin{aligned} &Q_{11} = Q_{21} = Q_{31} = (1-p)\varepsilon_1; \\ &Q_{42} = (1-p)\varepsilon_2; \\ &Q_{43} = p\varepsilon_1; \\ &Q_{14} = Q_{24} = Q_{34} = p\varepsilon_2; \end{aligned} \tag{3}$$

where $\varepsilon_1 = \exp[-2\pi i(2h + k)/3 - \varphi i]$, $\varepsilon_2 = \exp[-2\pi i\,(h + 2k)/3 - \varphi i]$, $\varphi = 2\pi[(\mathbf{s} - \mathbf{s}_0)/\lambda]\,\mathbf{c}$ and the other elements are zero. The characteristic equation of the $\mathbf{Q}$ matrix is given by

$$X^2[X^2 - (1-p)\varepsilon_1 X - p[p\varepsilon_1\varepsilon_2 + (1-p)\,\varepsilon_2^2] = 0. \tag{4}$$

As seen from the derivation of diffracted intensity by Kakinoki & Komura (1965), if both the characteristic equation of the difference equation and of the $\mathbf{Q}$ matrix multiplied by $\exp(\varphi i)$ are substantially equivalent to each other, the diffracted intensities calculated by the use of the difference equation and of matrix intensity equation become equal to each other. If we multiply (4) by $X - p\varepsilon_1\varepsilon_2 - (1-p)\,\varepsilon_2^2$ and put $\varphi = 0$, we obtain the same equation as (12) of Howard (1977).

Our method can be easily developed to the case where inserted layers are followed by another inserted layer with probability p' different from p. We denote complexions which follow with probability $1 - p'$ by $\mathbf{d}''_1$ and $\mathbf{d}''_2$ and those which follow with probability p' by $\mathbf{d}'''_1$ and $\mathbf{d}'''_2$. The probability tree for this case is shown in Fig. 1. When the complexions are numbered as follows,

$$\begin{aligned} &\mathbf{d}_1 = 1, \quad \mathbf{d}'_2 = 2, \quad \mathbf{d}''_2 = 3, \\ &\mathbf{d}''_1 = 4, \quad \mathbf{d}'''_1 = 5, \quad \mathbf{d}'''_2 = 6, \end{aligned} \tag{5}$$

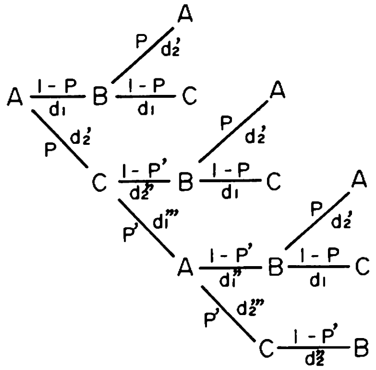

Fig. 1. Probability tree for $\mathbf{Q}$ matrix given by (6).

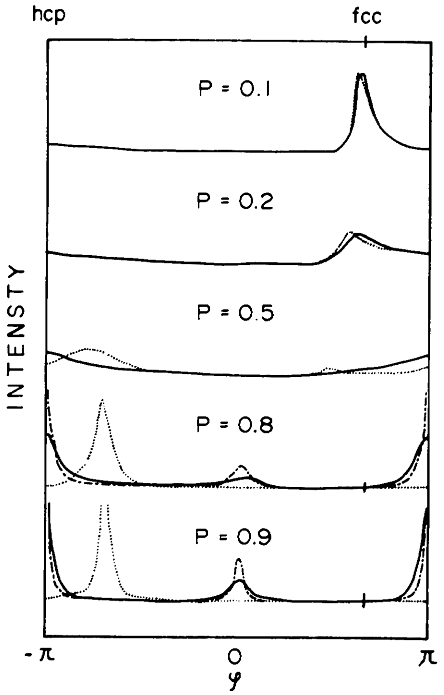

Fig. 2. Intensity profiles. Full line: $p = p'$. Broken line: $p' = 0$. Chain line: $1 - p' = \frac{1}{2}(1-p)$.

the elements of the **Q** matrix become:

$$\begin{aligned} &Q_{11}=Q_{31}=Q_{41}=(1-p)\varepsilon_1;\\ &Q_{12}=Q_{32}=Q_{42}=p\varepsilon_2;\\ &Q_{23}=Q_{63}=(1-p')\varepsilon_2;\\ &Q_{54}=(1-p')\varepsilon_1;\\ &Q_{25}=Q_{65}=p'\varepsilon_1;\\ &Q_{56}=p'\varepsilon_2; \end{aligned} \tag{6}$$

and the other elements are zero. The calculation of diffracted intensities with an electronic computer was programmed for the **Q** matrix given by (6). The **Q** matrix reduces to that of the first problem if $p'=0$, and to that of the second problem if $p=p'$. The calculated intensity profiles are shown in Fig. 2.

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References

HOWARD, C. J. (1977). *Acta Cryst.* A**33**, 29–32.
KAKINOKI, J. & KOMURA, Y. (1965). *Acta Cryst.* **19**, 137–147.
TAKAHASHI, H. (1976). *Bull. Fac. Educ. Univ. Kagoshima* (*Nat. Sci.*), **28**, 1–10.

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α, β and γ forms of *p*-dichlorobenzene: calculation of crystal structure and potential energy.

By K. MIRSKY and M. D. COHEN, *Department of Structural Chemistry, The Weizmann Institute of Science, Rehovot, Israel*

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A new potential function for non-bonded atom···atom interactions of chlorine atoms has been used to calculate equilibrium crystal structures and potential energies of the three polymorphs of solid *p*-dichlorobenzene.

There has been considerable interest in potential functions describing non-bonded atom···atom interactions of Cl atoms. Recently, we have introduced (Mirsky & Cohen, 1977) a new Cl···Cl potential function: this is of Buckingham form, $\varphi=-Ar^{-6}+B\exp(-\alpha r)$, with $A=2980$ Kcal mol^{-1}, $B=4580$ Kcal mol^{-1}, and $\alpha=2{\cdot}262$ Å^{-1}. Compared with other available potentials this has a large value (4·2 Å) of r_0, the minimum-energy interatomic distance, and is soft (the steepness parameter $\lambda=\alpha r_0=9{\cdot}5$). This function was successfully used for calculating the crystal structure parameters and lattice energies of a number of chloroaromatics, without additional terms to allow for electrostatic interactions.

One of the substances for which these calculations were performed was the γ form of *p*-dichlorobenzene (DCB). There are by now considerable structural data available on the three polymorphs of this compound. There have been studies at various temperatures of the monoclinic α phase [space group $P2_1/a$, $Z=2$ (Reynolds, Kjems & White, 1974; Wheeler & Colson, 1976; and references therein)], of the triclinic β phase [space group $P\bar{1}$, $Z=1$ (Reynolds *et al.*, 1974; Wheeler & Colson, 1976; and references therein)], and

Table 1. *β, α and γ phases of DCB: comparison of the calculated equilibrium unit-cell parameters with those extrapolated to* 0 K

	Polymorph								
	β			α			γ		
Unit-cell parameter*	Calculated	0 K	% theory/experiment	Calculated	0 K	% theory/experiment	Calculated	0 K	% theory/experiment
a (Å)	7·32	7·29	0·4	14·65	14·64	0	8·57	8·60	−0·4
b (Å)	5·75	5·85	−1·7	5·63	5·72	−1·6	5·98	6·00	−0·3
c (Å)	3·74	3·86	−3·2	3·83	3·90	−1·8	7·32	7·39	−1·0
α (°)†	91·8	90·9	0·9	90·0	90·0		90·0	90·0	
β (°)	109·7	112·4	−2·4	109·8	111·6	−1·6	127·3	127·5	−0·2
γ (°)†	94·1	92·7	1·5	90·0	90·0		90·0	90·0	
V_{mol} (Å^3)	147·9	151·9	−2·7	148·5	151·8	−2·2	149·2	151·3	−1·4

* The 0 K values for the β and α forms are found by extrapolation; those for the γ form are estimated with contractions of about 0·02 Å assumed in all cell dimensions between 100 and 0 K, as is found for β and α forms.

† For monoclinic space groups, only the monoclinic angle was varied.