Acta Cryst. (1974). A30, 39

X-ray Determination of the Mean-Square Atomic Displacements and Associated Debye Temperature of Mg_2Sn

BY E. F. SKELTON
U.S. Naval Research Laboratory, Washington, D.C. 20375, *U.S.A.*

AND S. T. LIN AND G. M. ROTHBERG
Stevens Institute of Technology, Hoboken, N.J. 07030, *U.S.A.*

(*Received* 16 *June* 1973; *accepted* 9 *August* 1973)

The mean-square atomic displacements and associated Debye temperature of Mg_2Sn have been determined from a least-squares analysis of 115 single-crystal X-ray scattering measurements. The mean-square displacements of Mg and Sn are 0·0138 (3) and 0·0097 (1) Å^2 respectively, and the corresponding Debye temperature is 270 ± 3 °K. The data have been analyzed in terms of possible anharmonic contributions to the thermal motion of the Mg atom. An analysis of published specific-heat data was performed to obtain the minus-second moment of the frequency spectrum. The Debye temperature associated with this moment, 281 ± 9 °K, is compared with the aforementioned X-ray value.

Introduction

Recent measurements of the Mössbauer absorption line of Sn^{119} in β-Sn have exhibited an explicit temperature dependence of the isomer shift (Rothberg, Guimard & Benczer-Koller, 1970). It has been inferred from this result that the electron density at the nucleus, $\psi^2(0)$, is temperature dependent, even at constant volume. Based on Knight-shift experiments in β-Sn, it is believed that the explicit temperature dependence of $\psi^2(0)$ is due to a possible interaction between the crystal lattice vibrations and the electrons at the Fermi surface. This phenomenon is not completely understood and, in an effort to test possible mechanisms, Mössbauer absorption spectra of β-Sn and Mg_2Sn were measured over a temperature range from 300 to 500 °K. The details of these measurements and the ensuing physical consequences are discussed elsewhere (Lin, Rothberg & Skelton, 1973).

However, in the work of Lin *et al.* (1973) the explicit temperature dependence of the isomer shift is compared with theoretical predictions based on a pseudopotential method. The temperature dependence of the pseudopotential is produced by modifying the form factors by the appropriate Debye–Waller factors and, in the case of Mg_2Sn, this treatment requires knowledge of the Debye–Waller factors for the Mg and Sn atoms. The experiment described in this paper was performed to provide this information.

Theory

The integrated intensity diffracted from an extended face of a mosaic crystal can be expressed as follows:

$$\varrho' = Cf(\theta)|F|^2 \qquad (1)$$

where C is a constant containing an unknown intensity scale factor, $f(\theta)$ is a known function of the Bragg diffraction angle only, and $|F|$ is the modulus of the structor factor. The structure factor for a fluorite-like lattice (space group $Fm3m$), such as Mg_2Sn, can be written, within the quasi-harmonic approximation, as follows:

$$F_{\rm cal} = 4\{f_{\rm Sn} \exp(-x\langle u^2_{\rm Sn}\rangle) + 2\delta_{hkl} f_{\rm Mg} \exp(-x\langle u^2_{\rm Mg}\rangle)\} \qquad (2)$$

$$F_{\rm cal} = 0 \quad \text{for mixed indices } (h,k,l)\dagger \qquad (3)$$

where

$$x = 8(\pi \sin\theta/\lambda)^2 \qquad (4)$$

and

$$\delta_{hkl} = \begin{cases} 0 \text{ for } h,k,l \text{ all odd} \\ +1 \text{ for } h+k+l=4n \\ -1 \text{ for } h+k+l=4n-2 \end{cases} n=1,2,3,\ldots \qquad (5)$$

The exponential terms in equation (2) represent the Debye–Waller factors for the two constituent atoms; $\langle u^2_{\rm Mg}\rangle$ and $\langle u^2_{\rm Sn}\rangle$ are the mean-square displacements of the two atoms parallel to the diffraction vector; $f_{\rm Mg}$ and $f_{\rm Sn}$ are the respective atomic scattering factors; all other terms have their standard meaning (as defined in *International Tables for X-ray Crystallography*, 1959).

In principle, the measured integrated intensities can be used to determine the three unknown parameters in the foregoing equations: values for the scale factor C and the two mean-square displacements are determined by a least-squares analysis of the measured integrated intensities as described below.

---

† We are grateful to the referee for pointing out the fact that Borie (1973) has recently shown that it is possible to thermally excite certain 'forbidden' Bragg reflections and therefore the equality of equation (3) may not be rigorously true.

Within the quasi-harmonic approximation, the mean-square displacements for this cubic, diatomic lattice are related to the frequency spectrum of the lattice $G(\omega)$ through the Debye–Waller theory as follows:

$$2m_{\rm Mg}\langle u^2_{\rm Mg}\rangle + m_{\rm Sn}\langle u^2_{\rm Sn}\rangle = \frac{3}{4\pi^2}\,\frac{\int G(\omega)\bar{E}(\omega)\omega^{-2}\mathrm{d}\omega}{\int G(\omega)\mathrm{d}\omega} \tag{6}$$

where $\bar{E}(\omega)$ is the mean energy of an oscillator of frequency ω, $m_{\rm Mg}$ and $m_{\rm Sn}$ are the respective atomic masses, and the integrations are performed over all frequencies (Blackman, 1956). If the Debye frequency distribution function is substituted for $G(\omega)$, the mean-square displacements can be expressed in terms of the X-ray Debye temperature Θ^M:

$$2m_{\rm Mg}\langle u^2_{\rm Mg}\rangle + m_{\rm Sn}\langle u^2_{\rm Sn}\rangle = 9\hbar^2 T[\Phi(\xi)+\xi/4]/[k(\Theta^M)^2] \tag{7}$$

where

$$\Phi(\xi) = \frac{1}{\xi}\int_{y=0}^{\xi} y(e^y-1)^{-1}\mathrm{d}y;\;\; \xi=\Theta^M/T. \tag{8}$$

Experimental procedure

The sample used for all X-ray measurements was provided by H. Lipson of the Air Force Cambridge Research Laboratory and grown from a stoichiometric melt by B. Lichter of Vanderbilt University, who also provided advice on handling techniques. It is in the approximate form of a rectangular platelet of dimensions $6\times2\times0{\cdot}5$ mm. The unit-cell parameter, a, was measured to be 6·7638 (4) Å which compares favorably with the published value of 6·7630 Å from the A.S.T.M. Powder Diffraction File (Card No. 7-274). The crystal mosaicity is characterized by the value of the Zachariasen (1967, 1969) extinction coefficient r^*, which was found to be $1{\cdot}2\times10^{-3}$ cm.

The largest face of the crystal is approximately parallel to the (111) planes. The sample was mounted on a Picker biplane diffractometer with its 111 diffraction vector approximately parallel to the χ-rotation axis, by the use of an Electronics and Alloys eucentric goniometer. All measurements were made from the large face of the sample and, by restricting the experiment to high diffraction angles ($2\theta\ge75°$), the incident X-ray beam was entirely intercepted by the crystal for all measurements. Those reflections within the aforementioned 2θ range having diffraction vectors closest to the 111 diffraction vector were selected for measurement.

The crystal was irradiated with filtered radiation from a Mo X-ray tube; the diffracted radiation was measured with a NaI(Tl) detector followed by a pulse-height discriminator. The intensity of each reflection was measured in the $\omega/2\theta$-scan mode over a range from 1·00° below the $K\alpha_1$ peak to 1·00° above the $K\alpha_2$ peak at a scanning speed of $\frac{1}{8}°$ min^{-1}. (The angular separation between the $K\alpha_1$–$K\alpha_2$ doublet ranged from 0·54° at 75° to 3·38° at 155°.) The angular height and width of the detector window were 1·25 and 0·73° respectively. The integrated intensities of 115 reflections were manually measured; these include 38 reflections with $(h+k+l)=4n$, 36 with $(h+k+l)=(4n-2)$ ($n=1,2,3,\ldots$), and 41 odd-index reflections.

Results and discussion

The relativistic Hartree–Fock atomic scattering-factor calculations of Doyle & Turner (1968), corrected for dispersion with Cromer's (1965) calculations, were used in analyzing the data. A number of corrections were applied to the measured integrated intensities. The correction for background scattering was made by the standard linear-extrapolation procedure. The relative standard deviation in the net intensity above background was less than 1% for all measurements and usually about $\frac{1}{2}$%. The data were also corrected for first-order acoustical-mode thermal diffuse scattering (TDS). The usual assumption was made that the smaller optic-mode and higher-order contributions to the TDS vary slowly under the Bragg peak and are therefore approximately accounted for in the background correction. The TDS correction was evaluated for all reflections using the procedure of Skelton & Katz (1968) and the elastic constant data of Davis, Whitten & Danielson (1967). The size of this correction varied from 5·7 to 11·1% over the range of reflections measured.

The measured intensities were corrected in the usual manner for the effects of absorption, polarization, and the Lorentz factor. A correction was also applied using the general formulas of Zachariasen (1967) to account for the effects of extinction. To evaluate this correction however, the mean radius of the crystallite domains and their relative misalignment must be known: these two parameters can be expressed in terms of a single constant, denoted as r^* by Zachariasen (1969). In addition foreknowledge of the results (in this case $\langle u^2_{\rm Mg}\rangle$ and $\langle u^2_{\rm Sn}\rangle$) is needed in order to calculate the structure factor and hence the extinction correction. The value of r^* was therefore included as an adjustable parameter in the general least-squares refinement program. The values of C, r^*, $\langle u^2_{\rm Mg}\rangle$, and $\langle u^2_{\rm Sn}\rangle$ were selected as those which yielded the best agreement, in the least-squares sense, between the 115 measured values of $F_{\rm obs}$ and the calculated structure factors, $F_{\rm cal}$. (The computer subroutine used to analyze the data was a modified version of program *E2 ANL FUNC* written by C. Chamot of Argonne National Laboratory.) The relative magnitude of the extinction correction is expected to decrease with increasing diffraction angle; in this case, it varied from about 4% to less than $\frac{1}{2}$% over the range of reflections measured.

Values of the mean-square displacements determined in this manner are: $\langle u^2_{\rm Mg}\rangle=0{\cdot}0138$ (3) and $\langle u^2_{\rm Sn}\rangle=0{\cdot}0097$ (1) Å^2. The estimated uncertainties are taken directly from the least-squares refinement program. A comparison of the values of F_{obs} and F_{cal} is shown in Fig. 1; the discrepancy index (R value) is 1·22%. (Incidently, it is interesting to note the similarity between these results and those reported by Cooper & Panke (1970) for the isomorphic compound Mg_2Si, *viz.* $\langle u^2_{\text{Mg}}\rangle = 0{\cdot}00968$ and $\langle u^2_{\text{Sn}}\rangle = 0{\cdot}00694$ Å^2. The ratio of mean-square displacements is 1·39 for Mg_2Si as compared with $1{\cdot}42 \pm 0{\cdot}05$ for Mg_2Sn, despite the obvious mass difference between Si and Sn.)† The value of $\langle u^2_{\text{Sn}}\rangle$ reported here agrees favorably with the room-temperature Mössbauer measurements on Mg_2Sn, *viz.* 0·0100 (8) Å^2, which is obtained after correcting the original result of Bryukhanov, Delyagin & Kuz'min (1964) for the more recent value of 5·5 for the Sn^{119} internal conversion coefficient (Muir, Ando & Coogan, 1966).

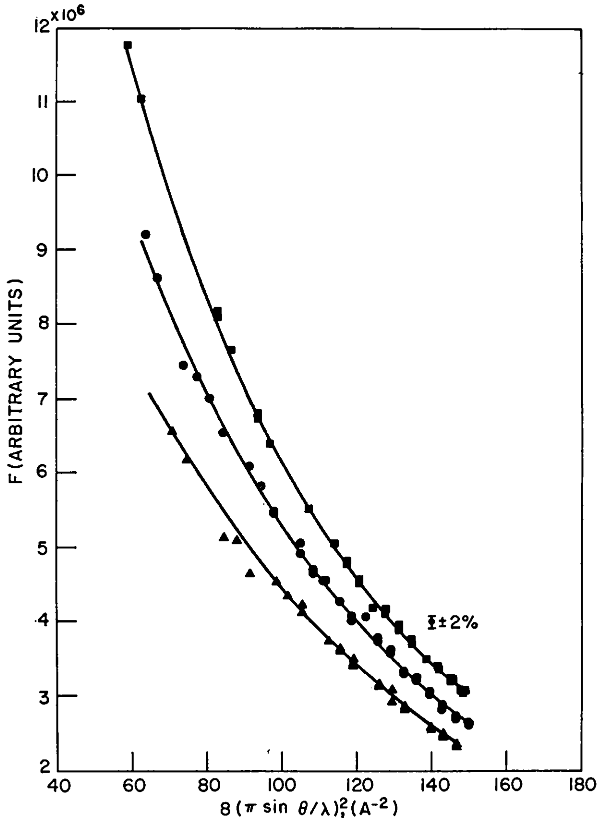

Fig. 1. Mg_2Sn structure factor *versus* $8(\pi \sin \theta/\lambda)^2$. ■ (h,k,l) all odd; ● $(h+k+l)=4n$; ▲ $(h+k+l)=4n-2$ ($n=1, 2, 3 \ldots$). Solid curves represent the calculated structure factors, F_{cal}.

We note that in several instances, systematic deviations between F_{obs} and F_{cal} have been observed in compounds with the fluorite structure, *viz.* UO_2 (Rouse, Willis & Pryor, 1968), CaF_2 (Willis, 1965; Strock & Batterman, 1972), and BaF_2 (Cooper, Rouse & Willis, 1968). Specifically, it is found that although agreement between F_{obs} and F_{cal} is usually within a few percent for the even-index data, systematic discrepancies are observed in the case of odd-index reflections, amounting to as much as ±60% for neutron scattering experiments on BaF_2 (Cooper *et al.*, 1968). In these instances, the discrepancies could be accounted for by assuming the atomic vibrations to be anisotropic and anharmonic.

Dawson, Hurley & Maslen (1967) have developed a phenomenological theory which permits evaluation of the structure factor for a fluorite lattice executing anharmonic thermal vibrations. [A more general version of this treatment has been presented by Willis (1969).] In the Dawson *et al.* theory, the solid is represented by an anharmonic Einstein model in that each atom is assumed to vibrate under the influence of a one-particle potential function. If this potential function is expanded about the equilibrium position of each atom in the unit cell and only terms to cubic order in the displacement are retained, then the motion of the anion in the above compounds will be anharmonic, whereas the cubic-order term appertaining to the cation will vanish. This results from the fact that, in this treatment, the form of the anharmonic term is dictated by the local site symmetry. (The anion in the above compounds is surrounded by four cations at the corners of a regular tetrahedron and occupies a non-centrosymmetric lattice site. The cation, on the other hand, is surrounded by eight anions located at the corners of a cube and is in a centrosymmetric position.)

Recently Cooper & Panke (1970) have noted that a similar situation exists in the case of Mg_2Si, although in this instance the discrepancies between F_{obs} and F_{cal} are generally less than a few percent. This compound, like Mg_2Sn, may be said to be 'anti-isomorphic' to the fluorite structure in that the more electronegative ion (Sn) occupies the usual cation position (Bryukhanov *et al.*, 1964). An effort was made to determine whether our data warranted a similar anharmonic treatment.

Since the details of the Dawson *et al.* (1967) theory have recently been reviewed by Strock & Batterman (1972), suffice it to say at this point that, within the framework of this treatment, the anharmonicity in Mg_2Sn is represented by the single constant β, *viz.* the third-order term in the expansion of the one-atom potential function for Mg about its equilibrium position. The parameter β is incorporated into the structure factor for the odd-index reflections in the following manner:

$$\delta_{hkl} = \mp \left[\frac{(hkl)\beta}{kT}\left\{\frac{2\pi}{a}\langle u^2_{\text{Mg}}\rangle\right\}^3\right] \quad \text{for } h+k+l=4n\pm 1\,. \tag{9}$$

---

† The referee has noted that this result is consistent with recent comments by Huiszoon & Groenewegen (1972) concerning the mass independence of the mean-square displacements at high temperatures. We wish to further point out that a serious criticism of this conclusion raised by Scheringer (1973), appears to be in error, as will be shown in a forthcoming paper by Feldman (1974).

In our analysis, we simply included the anharmonic correction in the general least-squares program and attempted to refine on the five parameters C, r^*, $\langle u^2_{Mg}\rangle$, $\langle u^2_{Sn}\rangle$, and β, simultaneously. It was discovered however, that the agreement between F_{obs} and F_{cal} was very insensitive to the value of β. A separate analysis was therefore carried out on the 41 odd-index reflections only; these reflections are expected to be the most sensitive to anharmonicity in this theory. The values of C, r^*, $\langle u^2_{Mg}\rangle$, and $\langle u^2_{Sn}\rangle$ were held fixed at their 'quasi-harmonic values' and a value for β was determined by a second least-squares analysis. We find that our data are best represented by a value of $-1{\cdot}2\times10^{12}$ erg cm^{-3} for β; however, because of the general insensitivity between F_{cal} and β in this instance, it would be prudent not to attach any physical significance to this result. The resulting R values for the quasi-harmonic and anharmonic treatments of the odd-index data are 1·45 and 1·24% respectively. According to Hamilton's (1965) significance test, this ratio of R values of 1·17 implies that the hypothesis separating the two calculations, *viz.* that anharmonicity is negligible in this case, can be rejected below the 0·5% confidence level, *i.e.* a purely quasi-harmonic treatment of the thermal motion of the Mg atoms appears to be inconsistent with our data.

However, it should also be pointed out that in our case, where the assumed anharmonic effects are only on the order of a few percent, it is possible that the differences noted above may arise from other approximations involved in our analysis, *e.g.* the assumption that the TDS is isotropic, the neglect of optic-mode and higher-order contributions to the TDS, or the occurrence of possible Renninger reflections. In any event, we do not expect that this will have any significant effect on our reported values for $\langle u^2_{Mg}\rangle$ and $\langle u^2_{Sn}\rangle$. As noted above, the apparent influence of anharmonicity on these terms is very small. Specifically, the general least-squares program was rerun including the anharmonic correction; the new values for $\langle u^2_{Mg}\rangle$ and $\langle u^2_{Sn}\rangle$ were found to be within the aforementioned error limits.

The mean-square displacements for Mg_2Sn can be combined in terms of an X-ray Debye temperature as indicated in equation (7). The value of Θ^M is found to be 270 ± 3°K. We realize that an uncertainty of ±1% is unusually small for an experimental X-ray determination of Θ^M and we again stress that these error limits are determined essentially from the least-squares refinement and that they include neither inaccuracies in the relative values of the atomic scattering factors, their angular dependence, nor uncertaintities in other parameters involved in the analysis of the data.

The value of Θ^M determined here compares very unfavorably with a value of 201°K reported by Bryukhanov *et al.* (1964). However, since the details of the X-ray experiment resulting in this 201°K value are unavailable to us, a critical comparison of these results is not possible.

Applying the procedure outlined by Barron, Leadbetter, Morrison & Salter (1966), we have analyzed the specific-heat data of Jelinek, Shickell & Gerstein (1967) and thereby determined the minus-second moment of the frequency spectrum. The Debye temperature associated with this moment may be compared directly with the value of Θ^M reported here. Based on the constant-volume specific heat values reported by Jelinek *et al.* (1967) and restricting our analysis to temperatures below 120°K (above 120° the specific-heat Debye temperature exhibits a strong temperature dependence which is inconsistent with the quasi-harmonic nature of the analysis), we find $\Theta^D(-2)$ to be about 283°K. We have been unable to locate low-temperature thermal expansion data for Mg_2Sn and therefore assumed the thermal expansivity to be proportional to the specific heat. On this basis, we estimate a relatively small volume-expansion correction to $\Theta^D(-2)$, *viz.* about -2°K. We therefore consider the value of Θ^M at high temperatures, as determined from the specific-heat data, to be about 281 ± 9°K. This value of Θ^M and our measured value of 270 ± 3°K are in satisfactory agreement considering the uncertainities involved.

Conclusion

In summary, we report here values for the mean-square displacements and the associated Debye temperature for Mg_2Sn, *viz.* $\langle u^2_{Mg}\rangle=0{\cdot}0138$ (3); $\langle u^2_{Sn}\rangle=0{\cdot}0097$ (1) Å^2; $\Theta^M=270\pm3$°K. We feel that our data are adequately represented within the usual quasi-harmonic theory and, although explicit anharmonic effects may be present, their influence on the aforementioned results is believed to be small. These results will be used in our evaluation of the temperature dependent Mössbauer data for Mg_2Sn which is to be reported elsewhere (Lin *et al.*, 1973).

References

BARRON, T. H. K., LEADBETTER, A. J., MORRISON, J. A. & SALTER, L. S. (1966). *Acta Cryst.* **20**, 125–131.

BLACKMAN, M. (1956). *Acta Cryst.* **9**, 734–737.

BORIE, B. S. (1973). *ACA Program & Abstracts*, paper B6, **1**, 124.

BRYUKHANOV, V. A., DELYAGIN, N. N. & KUZ'MIN, J. (1964). *J. Exp. Theor. Phys.* (*USSR*), **46**, 137–141. [*Sov. Phys. JETP*, **19**, 98–101].

COOPER, M. J., ROUSE, K. D. & WILLIS, B. T. M. (1968). *Acta Cryst.* A**24**, 484–493.

COOPER, M. J. & PANKE, D. (1970). *Acta Cryst.* A**26**, 292–293.

CROMER, D. T. (1965). *Acta Cryst.* **18**, 17–23.

DAVIS, L. C., WHITTEN, W. B. & DANIELSON, G. C. (1967). *J. Phys. Chem. Solids*, **28**, 439–447.

DAWSON, R. E., HURLEY, A. C. & MASLEN, V. W. (1967). *Proc. Roy. Soc.* A**298**, 289–306.

DOYLE, P. A. & TURNER, P. S. (1968). *Acta Cryst.* A**24**, 390–397.

Feldman, J. L. (1974). *Acta Cryst.* In the press.
Hamilton, W. C. (1965). *Acta Cryst.* **18**, 502–510.
Huiszoon, C. & Groenewegen, P. P. M. (1972). *Acta Cryst.* A**28**, 170–172.
International Tables for X-ray Crystallography (1959). Vol. II. Birmingham: Kynoch Press.
Jelinek, F. J., Shickell, W. D. & Gerstein, B. C. (1967). *J. Phys. Chem. Solids*, **28**, 267–270.
Lin, S. T., Rothberg, G. M. & Skelton, E. F. (1973). To be published.
Muir, A. H., Ando, K. J. & Coogan, H. M. (1966). *Mössbauer Effect Data Index* 1958–65. New York: Interscience.
Rothberg, G. M., Guimard, S. & Benczer-Koller, N. (1970). *Phys. Rev.* B**1**, 136–138.
Rouse, K. D., Willis, B. T. M. & Pryor, A. W. (1968). *Acta Cryst.* B**24**, 117–122.
Scheringer, C. (1973). *Acta Cryst.* A**29**, 82–86.
Skelton, E. F. & Katz, J. L. (1968). *Acta Cryst.* A**25**, 319–329.
Strock, H. B. & Batterman, B. W. (1972). *Phys. Rev.* B**5**, 2337–2343.
Willis, B. T. M. (1965). *Acta Cryst.* **18**, 75–76.
Willis, B. T. M. (1969). *Acta Cryst.* A**25**, 277–300.
Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564.
Zachariasen, W. H. (1969). *Acta Cryst.* A**25**, 102.

Acta Cryst. (1974). A**30**, 43

The Effect of Coordinate Errors on the Phase-angle Distribution*

By S. Parthasarathy and V. Parthasarathi
Centre of Advanced Study in Physics, University of Madras, Madras-600025, India

(*Received* 27 *June* 1973; *accepted* 10 *July* 1973)

The probability distribution of the magnitude of the phase-angle error ($|\theta^c|$) is worked out for an incomplete model structure when there are coordinate errors in the atomic positions. The corresponding problem for a centrosymmetric structure, namely the calculation of the percentage of reflexions for which the signs of the structure factors calculated from the coordinates of the model structure would agree with the true signs of the reflexions, is also worked out. The theoretical distributions could be used to study the effect of crystal-structure refinement on the phase-angle distribution. Numerical tables that are necessary for such a study are given.

Introduction

In an earlier paper (Parthasarathy, 1965*b*, hereafter referred to as P, 1965*b*) the probability distribution of θ,† which is the difference in the phase of the true structure factor F_N arising from all the N atoms in the unit cell and that due to the atoms from an incomplete model structure containing $P(<N)$ atoms, has been worked out under the assumption that there are no errors in the coordinates of the atoms of the model. However, the model structure that is met with at any stage in a crystal-structure analysis is such that there are random errors in the coordinates of the atoms of the model and the process of crystal structure refinement consists in reducing this error as much as possible, consistent with the amount and accuracy of the intensity data. In this connexion it would be interesting to study how the probability distribution of the phase-angle difference is modified as the errors in the coordinates of the atoms in the model are reduced. In this paper we shall work out the probability distribution of the phase-angle error θ^c which is the difference between the true phase of a reflexion and that (*i.e.* α_P^c) calculated from the coordinates of the atoms in the model structure. In order to avoid complications we shall consider only crystals and models which satisfy the requirements of the acentric distribution of Wilson (1949), namely the $P=MA$ case of P (1965*b*).

The corresponding problem for a centrosymmetric crystal would be (see Parthasarathy, 1965*a*, hereafter referred to as P, 1965*a*) the derivation of the probability function of s^c which is the product of the true sign s_N of the reflexion and that (*i.e.* s_P^c) calculated from the model structure. In this paper we shall also derive the probability function of s^c for crystals and models which satisfy the requirements of the centric distribution of Wilson (1949), namely the $P=M$ case of P (1965*a*).

Derivation of the probability distribution of θ^c

Consider a non-centrosymmetric crystal containing N atoms in the unit cell. Suppose that, at a given stage in a crystal-structure analysis, the model structure consists of $P(<N)$ atoms and let $\Delta\mathbf{r}_{Pj}$ be the error in the coordinates of atom j in the incomplete model. Following Luzzati (1952) we shall assume that the coordinate errors $\Delta\mathbf{r}_{Pj}$ $(j=1,2,\ldots P)$ are normally distributed independent random vectors and define the quantity D to be

$$D=\langle\cos 2\pi\mathbf{H}\,.\,\Delta\mathbf{r}\rangle_P \qquad (1)$$

---

* Contribution No. 364 from The Centre of Advanced Study in Physics, University of Madras, Madras-600025, India.

† θ is also the phase-angle error since it is the amount by which the phase α_P of the model structure (without coordinate errors) is to be increased in order to obtain the true phase α_N of the reflexion.