

Fig. 4 shows the  $R$  factor plotted against  $d^{*3}$ . Here the reflections were sorted into 20 spherical shells of equal volume, the outer limit of the outermost shell corresponding to  $(2 \sin \theta)/\lambda = 1 \cdot 0 \text{ \AA}^{-1}$ . Both these figures indicate that the three librational modes used are highly effective in reducing the  $R$  factor, suggesting that the variation in  $B$  between the surface and the interior of the molecule is the predominant systematic variation of this quantity. No optimization has been done in which the model included the internal modes and the translations, to the exclusion of the librations.

Finally, in Fig. 5 we show stereo pairs of *ORTEP* drawings (Johnson, 1976) of the  $\alpha$ -carbon atoms alone. It is noticeable that internal and bridged residues, such as Phe 22 and Cys 55, have closely similar almost spherical distributions which are dominated by the lattice contribution. Other regions, especially the termini, show marked elongations with a tendency for the major axis of each ellipsoid to be transverse to its position vector relative to the molecular centre. The portion of chain from Gly 37 to Arg 42 also shows substantial anisotropy with the elongation largely transverse to the length of the chain. Lateral movements of this portion correspond to soft deformations of the molecule and to displacements as between form I and form II of this molecule (Wlodawer, Deisenhofer & Huber, 1987).

## References

- BERNSTEIN, F.C., KOETZLE, T.F., WILLIAMS, G.J.B., MEYER, E.F. JR, BRICE, M.D., RODGERS, J.R., KENNARD, O., SHIMANOCHI, T. & TASUMI, M. (1977). *J. Mol. Biol.* **112**, 535–542.
- DIAMOND, R. (1976). In *Crystallographic Computing Techniques*, edited by F.R. AHMED, pp. 291–301. Munksgaard: Copenhagen.
- EDWARDS, C., PALMER, S.B., EMSLEY, P., HELLIWELL, J.R., GLOVER, I.D., HARRIS, G.W. & MOSS, D.S. (1990). *Acta Cryst.* **A46**, 315–320.
- HAMILTON, W.C. (1959). *Acta Cryst.* **12**, 609–610.
- HENDRICKSON, W.A. & KONNERT, J.H. (1981). In *Biomolecular Structure, Conformation, Function and Evolution*, edited by R. SRINIVASAN, pp. 43–58. Oxford: Pergamon.
- HOWLIN, B., MOSS, D.S. & HARRIS, G.W. (1989). *Acta Cryst.* **A45**, 851–861.
- International Tables for X-ray Crystallography* (1968). Vol. III. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- JOHNSON, C.K. (1976). *ORTEP II. A Fortran Thermal Ellipsoid Plot Program for Crystal Structure Illustrations*. Report ORNL-5138, Oak Ridge National Laboratory, Tennessee, USA.
- KONNERT, J.H. & HENDRICKSON, W.A. (1980). *Acta Cryst.* **A36**, 344–350.
- LEVITT, M., SANDER, C. & STERN, P.S. (1985). *J. Mol. Biol.* **181**, 423–447.
- SCHOMAKER, V. & TRUEBLOOD, K.N. (1968). *Acta Cryst.* **B24**, 63–76.
- STERNBERG, M.J.E., GRACE, D.E.P. & PHILLIPS, D.C. (1979). *J. Mol. Biol.* **130**, 231–253.
- WLODAWER, A., DEISENHOFER, J. & HUBER, R. (1987). *J. Mol. Biol.* **193**, 145–156.
- WLODAWER, A., WALTER, J., HUBER, R. & SJÖLIN, L. (1984). *J. Mol. Biol.* **180**, 301–329.

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## Temperature Factor of Silicon by Powder Neutron Diffraction

BY ZHANG BAISHENG, YANG JILIAN, JIN LAN AND YE CHUNTANG

*Institute of Atomic Energy, PO Box 275 (30), Beijing, People's Republic of China*

AND J. BASHIR, N. M. BUTT,\* M. SIDDIQUE, M. ARSHED AND Q. H. KHAN

*Pakistan Institute of Nuclear Science and Technology, PO Nilore, Islamabad, Pakistan*

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### Abstract

The temperature factor of silicon has been determined by the powder neutron diffraction technique employing a double-axis neutron diffractometer. A neutron wavelength of  $1.184 \text{ \AA}$  was used in the experiment. The sample used was a fine powder of silicon of purity 99.999%. The correction to the observed intensities due to thermal diffuse scattering (TDS) was not applied as the neutron velocity of  $3.34 \text{ km s}^{-1}$  (corresponding to neutron wavelength of  $1.184 \text{ \AA}$ ) is less

than the minimum velocity of sound in this crystal. The  $B$  value obtained from these experiments was found to be  $0.45 (2) \text{ \AA}^2$ , corresponding to a mean-square vibrational amplitude of  $0.017 (2) \text{ \AA}^2$  and to a Debye temperature of  $531 (11) \text{ K}$  at the sample temperature of  $284 \text{ K}$  at which the experiment was performed.

### Introduction

Silicon is an important element of commercial interest and accurate measurement of its physical properties is desirable. One such physical parameter is the total

\* To whom all correspondence should be addressed.

mean-square amplitude of atomic vibrations  $\langle U^2 \rangle$  which, for a cubic structure, is related to the temperature factor  $B$  by

$$B = 8\pi^2/3 \langle U^2 \rangle.$$

Several authors have measured the temperature factor  $B$  of silicon employing various methods such as X-ray powder diffraction (Gottlicher & Wolfel, 1959; Batterman & Chipman, 1962), X-ray single-crystal diffraction (Batterman, 1962; Giardina & Merlini, 1973), neutron single-crystal diffraction (Graf, Schneider, Freund & Lehmann, 1981) and using the critical-voltage effect in high-voltage electron diffraction (HVED) (Eguchi, Tomokiyo & Matsuhata, 1987). Reichelt & Rodgers (1966) and Izumi, Asano, Murata & Watanabe (1987) determined the temperature factor of silicon by the time-of-flight (TOF) neutron scattering technique on powder samples.

While there is good agreement among the values obtained by X-ray diffraction methods, there is a large discrepancy (much beyond the experimental error) between the two values using the neutron powder TOF method referred to above. Furthermore, no investigation of the  $B$  value of silicon using a fixed-wavelength neutron powder diffractometer (an accurate method for such a determination) has been carried out. Therefore it was desirable to make diffraction measurements on a pure sample of silicon, using such a neutron powder diffractometer. In addition to resolving the discrepancy, these data provide support to the Temperature Factor Compilation Project of the Neutron Diffraction Commission of the International Union of Crystallography (Butt, Heger & Willis, 1985).

### Experimental

The neutron-diffraction experiment was performed on the double-axis neutron diffractometer installed at the 15MW Heavy Water Research Reactor of the Institute of Atomic Energy, Beijing, China. (200) planes of a pyrolytic graphite monochromator were used as reflecting planes, which gave a neutron wavelength of 1.184 Å. The flux of monochromated neutrons incident at the sample was about  $10^9$  neutrons  $m^{-2} s^{-1}$ . Silicon powder of purity 99.999% and particle size 50  $\mu m$  was contained in a thin-walled vanadium container of 1 cm diameter and 5 cm length. Data were collected over an angular range of  $2\theta$  from 20 to about  $117^\circ$  with a step of  $0.15^\circ$ . The neutron diffraction intensity at each step was recorded for the time interval determined by the preset monitor counts. All measurements were carried out at the ambient temperature of 284 K.

### Results and discussion

The observed ( $I_{obs}$ ) and calculated ( $I_{cal}$ ) intensities of the individual peaks obtained are given in Table

Table 1. *Observed and calculated intensities for silicon powder*

$hkl$	$I_{obs}$	$I_{cal}$
111	27 702	27 967
220	30 144	30 195
311	22 883	22 534
400	7 940	7 960
331	12 615	12 720
422	20 008	20 609
511, 333	12 812	12 371
440	7 478	7 619
531	14 130	14 149
620	12 160	12 733
533	6 673	6 036
444	4 090	3 739
711, 511	11 179	10 630
642	20 191	20 027
731, 553	14 635	14 821

Table 2. *The temperature factor  $B$  of silicon as determined by various authors*

$B$ (Å <sup>2</sup> )	$\Theta_D$ (K)	$T$ (K)	Method	Reference
0.45	545	300	XRP	(a)
0.44 (1)	543 (8)	291	XRP	(b)
0.47 (1)	530 (4)	298	XRP	(c)
0.46	538	300	XRP	(d)
0.32	658	300	NDP, TOF	(e)
0.48 (4)	522 (22)	295	NDP, TOF	(f)
0.45 (3)	545 (20)	300	XRSC	(g)
0.48 (1)	521 (5)	291	XRSC	(h)
0.45 (1)	539 (6)	295	NDSC	(i)
0.49	518	298	HVED	(j)
0.45 (2)	531 (11)	284	NDP	(k)

Notes: XRP=X-ray powder; XRSC=X-ray single crystal; NDP=neutron diffraction powder; TOF=time-of-flight method; NDSC=neutron diffraction single crystal; HVED=high-voltage electron diffraction; T=temperature of measurement.

References: (a) Gottlicher & Wolfel (1959); (b) Batterman & Chipman (1962); (c) Volland, Deus & Schneider (1976); (d) Glazer, Hidaka & Bordas (1978); (e) Reichelt & Rodgers (1966); (f) Izumi, Asano, Murata & Watanabe (1987); (g) Batterman (1962); (h) Giardina & Merlini (1973); (i) Graf, Schneider, Freund & Lehmann (1981); (j) Eguchi, Tomokiyo & Matsuhata (1987); (k) present work.

1. The final  $R$  value was 1.98% which indicates good reliability of the data. The observed intensities need not be corrected for TDS as the neutron velocity (3.34  $km s^{-1}$  corresponding to neutron wavelength of 1.184 Å) was smaller than the minimum sound velocity (4.67  $km s^{-1}$ ) in silicon. The sound velocity in silicon was calculated using the elastic-constants data of Parsad & Wooster (1955). In such a situation, the first-order TDS contribution to the Bragg peaks is zero (Willis, 1969). However, in several materials the intensities should be corrected for contributions due to TDS which may lead to a correction to the  $B$  value by a few percent.

The temperature factor  $B$  determined in this way in the present experiment is compared with the results of other authors in Table 2. The present value of  $B$  is 0.45 (2) Å<sup>2</sup> and corresponds to a Debye temperature  $\Theta_D$  of 531 (11) K, which is in good agreement with X-ray diffraction results (Gottlicher & Wolfel, 1959; Batterman & Chipman, 1962; Glazer, Hidaka & Bordas, 1978), and the neutron diffraction

single-crystal work of Graf, Schneider, Freund & Lehmann (1981).

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#### References

- BATTERMAN, B. W. (1962). *Phys. Rev.* **127**, 686-690.  
 BATTERMAN, B. W. & CHIPMAN, D. R. (1962). *Phys. Rev.* **127**, 690-963.  
 BUTT, N. M., HEGER, G. & WILLIS, B. T. M. (1985). *Acta Cryst.* **B41**, 374.  
 EGUCHI, T., TOMOKIYO, Y. & MATSUHATA, H. (1987). *J. Microsc. Spectrosc. Electron.* **12**, 559-568.  
 GIARDINA, M. D. & MERLINI, A. (1973). *Z. Naturforsch. Teil A*, **28**, 1360-1365.  
 GLAZER, A. M., HIDAKA, M. & BORDAS, J. (1978). *J. Appl. Cryst.* **11**, 165-172.  
 GOTTLICHER, V. S. & WOLFEL, E. (1959). *Z. Elektrochem.* **63**, 891-901.  
 GRAF, H. A., SCHNEIDER, J. R., FREUND, A. K. & LEHMANN, M. S. (1981). *Acta Cryst.* **A37**, 863-871.  
 IZUMI, F., ASANO, H., MURATA, H. & WATANABE, N. (1987). *J. Appl. Cryst.* **20**, 411-418.  
 PARSAD, S. C. & WOOSTER, W. A. (1955). *Acta Cryst.* **8**, 361.  
 REICHELTER, J. M. A. & RODGERS, A. L. (1966). *Nucl. Instrum. Methods*, **45**, 242-245.  
 VOLAND, U., DEUS, P. & SCHNEIDER, H. A. (1976). *Phys. Status Solidi A*, **36**, K165-K169.  
 WILLIS, B. T. M. (1969). *Acta Cryst.* **A25**, 277-300.

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## Elastic Coefficients of Polychromatic Crystals

BY K. RAMA MOHANA RAO\*

*Department of Applied Mathematics, AUPG Extension Centre, Nuzvid 521201, Andhra Pradesh, India*

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### Abstract

The group-theoretical method of reducing the polar (axial) tensor representation of the full rotation group has been explored and extended to obtain the second-, the third- and the fourth-order elastic coefficients for the 18 polychromatic crystal classes. The elastic coefficients obtained for all the classes are tabulated and the results obtained are briefly discussed.

### 1. Introduction

Many significant contributions on the study of the physical properties of crystals have been brought to light by several group-theoretical physicists during the past few decades. The number of non-vanishing as well as independent constants for the various physical properties in respect of the 32 conventional crystal classes were derived in considerable detail using group-theoretical as well as tensor methods by Bhagavantam & Venkatarayudu (1951), Wooster (1979), Nye (1985) and others. The book by Bhagavantam (1966) enhances the use of the character method in studying the magnetic properties of

these 32 classes and the 58 magnetic (double-colour) point groups derived from them. In two of the earlier papers published by the author (Rama Mohana Rao, 1987, 1988) the 18 applicationally significant polychromatic crystal classes (Indenbom, Belov & Neronova, 1960) were studied for three identified magnetic properties such as piezomagnetism and for six physical properties such as photoelasticity. The number of independent constants ( $n_i$ ) required to describe a chosen magnetic/physical property was obtained using a group-theoretical procedure also established by the author (Rama Mohana Rao, 1987).

It is well known that the physical property of elasticity describes the relation between the stress field developed and the strains caused. Further, the applied stress as well as the resulting strain could be represented by second-rank symmetric tensors. Bhagavantam & Suryanarayana (1949) and Jahn (1949) successfully enumerated the second- and third-order elastic coefficients for the 32 conventional crystal classes employing group-theoretical methods. With a slightly different approach to the application of the character method, following a suggestion made by Chelam (1961), Krishnamurty (1963) and Krishnamurty & Gopala Krishna Murty (1968) also derived these coefficients for the 32 conventional crystal classes.

\* Junior Associate Member at the International Centre for Theoretical Physics (ICTP), Trieste, Italy.