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Debye–Waller Factors and Debye Temperature of ZnTe

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Dedicated to Professor R. M. Chaudhri, Professor Emeritus, Punjab University, Lahore, Pakistan, on his 85th birthday

Abstract

Accurate measurements were made to determine the Debye temperature and Debye–Waller factors for powder ZnTe by the method of elastic neutron diffraction, using a triple-axis neutron spectrometer. Measurements were made with neutrons of wavelength 1·17 Å and corrections were made for the thermal diffuse scattering. The values of the Debye–Waller factors are $B_{\rm Zn} = 1{\cdot}26(5)$ and $B_{\rm Te} = 0{\cdot}74(5)$ Å^2. The mass-weighted mean value $\bar{B}$ is 0·91(5) Å^2 which corresponds to a Debye temperature $\Theta = 198(5)$ K. The results are in good agreement with the values determined by Cooper, Rouse & Fuess [*Acta Cryst.* (1973), A29, 44-56] using single-crystal neutron diffraction techniques.

Introduction

The Debye–Waller coefficient $\bar{B}$ for ZnTe has been obtained by many workers using X-ray diffraction (Blattner, Walford & Baldwin, 1972; Yamanaka & Tokonami, 1985), neutron diffraction (Cooper, Rouse & Fuess, 1973), inelastic neutron scattering [Vagelatos, Wehe & King, 1974) and Mössbauer absorption (Balciuniene, Dragunas & Makariunas, 1979). The B values have also been calculated from various theoretical lattice-dynamical models (Vetelino, Gaur & Mitra, 1972; Talwar & Agrawal, 1974; Plumelle & Vandevyver, 1976).

Although there is good agreement between the X-ray and Mössbauer absorption results, there is, in general, a disagreement between the X-ray and neutron diffraction results. In fact B values determined by the single-crystal neutron diffraction method (Cooper *et al.*, 1973) are some 20% lower than the B values determined from measured phonon density of states (Vagelatos *et al.*, 1974). Also, no explicit investigation of the Debye–Waller factors and Debye temperature of ZnTe by the powder neutron diffraction method has been reported. We therefore took up the study of these parameters for the cubic phase (at room temperature) of ZnTe by the powder neutron diffraction method. The data of this experiment are of interest to the IUCr project on compilation of temperature factors of cubic elements and compounds (International Union of Crystallography, 1985).

Theory

The space group of the cubic (zinc-blende) phase is $F\bar{4}3m$. The structure factors in this case can be expressed in three forms of the sum of h, k and l related to $4n$, $4n \pm 1$, or $4n \pm 2$, n being an integer. With Zn atoms at $(0, 0, 0)$ and equivalent positions and Te atoms at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ and equivalent positions, the structure factors are given by

$$F^2_{4n} = 16[b_{\rm Zn} \exp(-M_{\rm Zn}) + b_{\rm Te} \exp(-M_{\rm Te})]^2 \quad (1)$$

for $h+k+l = 4n$, $n = 1, 2, \ldots$;

$$F^2_{4n\pm1} = 16[b_{\rm Zn} \exp(-M_{\rm Zn})]^2 + 16[b_{\rm Te} \exp(-M_{\rm Te})]^2 \quad (2)$$

for $h+k+l = 4n \pm 1$; and

$$F^2_{4n+2} = 16[b_{\rm Zn} \exp(-M_{\rm Zn}) - b_{\rm Te} \exp(-M_{\rm Te})]^2 \quad (3)$$

for $h+k+l = 4n+2$, where $M = B\ [(\sin^2\theta)/\lambda^2]$, B being the Debye–Waller coefficient, $b_{\rm Zn}$ ($= 5{\cdot}8$ fm) and $b_{\rm Te}$ ($= 5{\cdot}7$ fm) are the neutron scattering lengths of Zn and Te atoms respectively (Bacon, 1975). As the neutron scattering lengths of Zn and Te atoms are nearly equal, reflections of the $4n+2$ type were weak and could not be measured.

From (1) and (2), we can write (Butt, Rouse & Thomas, 1978)

$$\ln(\alpha+\beta) = \text{constant} - B_{\rm Zn} (\sin^2\theta)/\lambda^2 \quad (4)$$

$$\ln(\alpha-\beta) = \text{constant} - B_{\rm Te} (\sin^2\theta)/\lambda^2 \quad (5)$$

where

$$\alpha = [F^2_{4n}]^{1/2} \quad \text{and} \quad \beta = [2F^2_{4n\pm1} - F^2_{4n}]^{1/2}. \quad (6)$$

Thus the plots of $\ln(\alpha+\beta)$ and $\ln(\alpha-\beta)$ *vs* $(\sin^2\theta)/\lambda^2$ will be straight lines; the slopes of these two straight lines yield $B_{\rm Zn}$ and $B_{\rm Te}$ respectively.

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Experimental procedure and data analysis

Fine ZnTe powder of purity 99·9% was sealed in a 2 cm diameter and 5 cm high cylindrical vanadium container. The triple-axis neutron spectrometer TKSN-400 installed at the PINSTECH 5 MW research reactor was used to measure the diffraction pattern. (220) planes of a copper single crystal and (200) planes of pyrolytic graphite were used as monochromator and analyser respectively at a neutron wavelength of 1·17 Å. The Soller collimation used before and after the sample was 30 and 40′ respectively. Four odd-order and five even-order reflections up to 620 were measured. The structure factors were evaluated from the diffraction data in the usual manner (Bacon, 1975) and α and β were calculated from (6).

Calculations were performed to evaluate the percentage thermal diffuse scattering (TDS) error under the Bragg peak according to Beg, Aslam, Butt, Khan & Rolandson (1974). For the TDS calculations an isotropic value of the sound velocity according to the model of Nilsson (1957) was used, employing the elastic constants given by Lee (1970). The TDS error varied from 0·1% for the 111 reflection to 1·8% for the 620 reflection. The correction to the B value due to TDS was therefore found to be small and was within experimental errors.

B_{Zn} and B_{Te} were obtained by a least-squares fit to (4) and (5). The experimental results were $B_{\mathrm{Zn}} = 1{\cdot}26(5)$, $B_{\mathrm{Te}} = 0{\cdot}74(5)$ Å^2 and the mass-weighted average value $\bar{B} = 0{\cdot}91(5)$ Å^2, corresponding to a Debye temperature of 198(5) K. The theoretical structure factors F_c were calculated by a standard procedure using a model with only the scale factor and the temperature factor $\bar{B}$ as refinable parameters. The observed and calculated structure factors corrected for TDS are compared in Table 1, which also shows the calculated TDS correction for each reflection. The R value for the fit was 0·5%, which indicates good agreement between the measured and calculated structure factors.

The results of previous experimental and theoretical determinations of thermal parameters at room temperature are summarized in Table 2. The average value of $\bar{B}$ from the literature is 0·89 Å^2, which is in good agreement with our value. The present values are also in close agreement with those of Cooper *et al.* (1973) determined by the single-crystal neutron diffraction method.

Table 1. *Observed and calculated structure factors and the TDS correction for ZnTe at room temperature*

hkl	F_o	F_c	TDS (%)
111	6·04	6·04	0·1
220	7·79	7·78	0·3
311	5·71	5·74	0·4
400	7·41	7·42	0·7
331	5·53	5·46	0·8
422	7·04	7·07	1·1
440	6·71	6·74	1·4
531	4·93	4·94	1·5
620	6·48	6·42	1·8

Table 2. *Room-temperature B values for* ZnTe

B_{Zn} (Å^2)	B_{Te} (Å^2)	$\bar{B}$ (Å^2)	Θ (K)	Method	Reference
		1·07(6)	182(5)	XRP	Blattner *et al.* (1972)
1·33	0·92	1·06	183	XRSC	Yamanaka & Tokonami (1985)
1·296(34)	0·758(11)	0·94(3)	194(2)	NDSC	Cooper *et al.* (1973)
		0·66	234	PHDR	Vagelatos *et al.* (1974)
		1·14(8)	178(6)	MABS	Balciuniene *et al.* (1979)
0·734	0·725	0·73	222	TH	Vetelino *et al.* (1972)
1·239	1·239	1·239	171	TH	Talwar & Agrawal (1974)
		0·54	260	TH	Plumelle & Vandevyver (1976)
1·26(5)	0·74(5)	0·91(5)	198(5)	NDP	Present work

Abbreviations

XRP: X-ray powder.
XRSC: X-ray single crystal.
NDSC: Neutron diffraction single crystal.
PHDR: Phonon dispersion relation (inelastic neutron scattering).
MABS: Mössbauer absorption.
TH: Theoretical.
NDP: Neutron diffraction powder.

References

BACON, G. E. (1975). *Neutron Diffraction.* Oxford: Clarendon Press.

BALCIUNIENE, M. L., DRAGUNAS, A. K. & MAKARIUNAS, K. V. (1979). *Sov. Phys. Crystallogr.* **19**, 68–73.

BEG, M. M., ASLAM, J., BUTT, N. M., KHAN, Q. H. & ROLANDSON, S. (1974). *Acta Cryst.* **A30**, 662–667.

BLATTNER, R. J., WALFORD, L. K. & BALDWIN, T. O. (1972). *J. Appl. Phys.* **43**, 935–938.

BUTT, N. M., ROUSE, K. D. & THOMAS, M. W. (1978). *Acta Cryst.* **A34**, 759–761.

COOPER, M. J., ROUSE, K. D. & FUESS, H. (1973). *Acta Cryst.* **A29**, 44–56.

INTERNATIONAL UNION OF CRYSTALLOGRAPHY (1985). *Acta Cryst.* **B41**, 374.

LEE, B. H. (1970). *J. Appl. Phys.* **41**, 2984–2987.

NILSSON, N. (1957). *Ark. Fys.* **12**, 247–257.

PLUMELLE, P. & VANDEVYVER, M. (1976). *Phys. Status Solidi B*, **73**, 271–281.

TALWAR, D. N. & AGRAWAL, B. K. (1974). *J. Phys. C*, **7**, 2981–2987.

VAGELATOS, N., WEHE, D. & KING, J. S. (1974). *J. Chem. Phys.* **60**, 3613–3618.

VETELINO, J. F., GAUR, S. P. & MITRA, S. S. (1972). *Phys. Rev. B*, **5**, 2360–2366.

YAMANAKA, T. & TOKONAMI, M. (1985). *Acta Cryst.* **B41**, 298–304.