Acta Cryst. (1980). A**36**, 147–148

The Debye–Waller Parameter ($\bar{B}$) of TlCl by Powder Elastic Neutron Diffraction

BY S. MAHMOOD, N. M. BUTT, N. AHMED, M. M. BEG, Q. H. KHAN AND J. ASLAM

Pakistan Institute of Nuclear Science and Technology, PO Nilore, Rawalpindi, Pakistan

(*Received* 26 *April* 1979; *accepted* 30 *August* 1979)

Abstract

The mean Debye–Waller parameter $\bar{B}$ of TlCl has been determined by double- as well as triple-axis neutron diffraction for a powder sample. Thermal diffuse scattering (TDS) corrections have also been made to the intensity of the diffraction peaks obtained by these techniques. TDS was found negligible in the triple-axis diffraction pattern as expected. The '$\bar{B}$' values thus found are $3{\cdot}08 \pm 0{\cdot}43$ and $3{\cdot}07 \pm 0{\cdot}22$ Å^2, respectively, for double- and triple-axis methods. These values are in good agreement with those found by recent X-ray diffraction measurements.

1. Introduction

Thalium chloride (TlCl) is a substance with CsCl-type structure with lattice constant $a = 3{\cdot}834$ Å. It is of current interest for studies regarding atomic vibrations because of the large difference in the masses of Tl and Cl (^{m}Tl/^{m}Cl = 5·77). In this connection, Haav, Peljo & Sourtti (1977) have observed that the heavier atom has a larger amplitude of vibration compared to the lighter atom ($B_{Tl} = 3{\cdot}39$ and $B_{Cl} = 2{\cdot}09$ Å at room temperature) which is not normally the case. This effect has also been observed in some other materials by Korhonen & Linkoaho (1966), Sanger (1969), Raccah & Arnott (1967), Groenewegen & Huiszoon (1972) and Jex, Müllner & Dyck (1974). Theoretical consideration of this aspect is also given in Willis & Pryor (1975).

Further, Bats (1976) has observed that in some materials considerable discrepancies exist in the thermal parameters, B, measured by X-ray and neutron diffraction techniques. Therefore, an interest exists to determine this parameter by neutron diffraction even though it has already been determined by X-ray diffraction.

An extensive experimental study for the determination of the parameter 'B' has already been done using powder X-ray diffraction by Myuirsepp & Khaav (1976) and Haav, Peljo & Sourtti (1977). The B values of TlCl have also been calculated by Joshi & Mitra (1960) and then by Gluyas, Hunter & James (1975), using the data of elastic constants, but their calculated values differ considerably between themselves, in addition to a large discrepancy between the experimental values of the X-ray work of Haav, Peljo & Sourtti (1977) and our neutron diffraction results. This is clear from Table 1. However, no neutron diffraction study of the B values of TlCl has been made so far; we have therefore taken up experimental investigation of this parameter for TlCl using neutron diffraction techniques, in particular using the high-resolution, three-axis elastic diffraction used by us in our earlier experiments (Beg *et al.*, 1974; Butt *et al.*, 1976; Ahmed *et al.*, 1977). In the triple-axis mode of diffraction, the thermal diffuse scattering (TDS) correction is very small (Caglioti, 1964).

2. Experimental procedure and data analysis

TlCl powder was ground (with particle size less than 80 μm) and sealed in a vanadium container. The triple-axis neutron spectrometer TKSN-400 installed at the 5 MW research reactor at PINSTECH was used to measure the diffraction pattern. A Cu (220) single crystal and graphite (004) were used as monochromator and analyser, respectively, at the neutron wavelength of 1·07 Å.

For the triple-axis mode, thermal diffuse scattering (TDS) correction to the observed intensities given in

Table 1. *Debye temperature values for* TlCl

Reference	$\bar{B}_{TlCl}$ (Å^2)	θ (K)	Method
Joshi & Mitra (1960)	1·80	125	Calculated from elastic constants
Gluyas *et al.* (1975)		141	Calculated from elastic constants
Myuirsepp & Khaav (1976)	2·86	101	By X-ray diffraction at room temperature
Haav *et al.* (1977)	3·20	95	By X-ray diffraction at room temperature
Present work	$3{\cdot}07 \pm 0{\cdot}22$	$97 \pm 3{\cdot}5$	Triple-axis } neutron diffraction at room temperature
	$3{\cdot}08 \pm 0{\cdot}43$	97 ± 7	Double-axis }

0567-7394/80/010147-$01.00

Table 2 was made as in Beg *et al.* (1974) and Beg (1976). Elastic constants of TlCl given by Gluyas, Hunter & James (1975) were used to find the isotropic sound velocity for the thermal diffuse scattering calculations. The spectrometer was used in the focusing mode. The angular resolution (*i.e.* full width at half maximum divided by the scattering angle) was almost the same throughout the spectrum and was of the order of 1%.

In the double-axis pattern, the observed intensities as given in Table 3 were corrected for TDS by the method of Chipman & Paskin (1959). Since only the acoustic modes contribute to the TDS, whereas both the acoustic and optic modes contribute to the Debye–Waller factor, the value of $\bar{B}$ used in the calculation of the TDS correction was $\frac{2}{3}\bar{B}$ (Sourtti, 1967), where $\bar{B}$ is the average value for the two atoms.

3. Results and discussion

The Debye–Waller parameter $\bar{B}$ for TlCl was calculated from the measured data of $h + k + l = 2n$ type of peaks in the harmonic approximation. The neutron scattering amplitudes of Tl and Cl differ by about 10%, therefore the intensities of the reflections with $h + k + l = 2n \pm 1$ will largely be caused by the difference of the b values of Tl^+ and Cl^-. Hence these reflections are very weak and need not be determined very exactly to get significant information about the individual temperature factors. Therefore only average $\bar{B}$ values of TlCl were found.

Table 2. *Observed integrated intensities using triple-axis mode*

$h\,k\,l$	Intensity
1 1 0	16796
2 0 0	3556
2 1 1	7114
2 2 0	2519
3 1 0	2808
3 2 1	3883
4 2 0	634

Table 3. *Observed integrated intensities using double-axis mode*

$h\,k\,l$	Intensity
1 1 0	44397
2 0 0	6388
2 1 1	16127
2 2 0	5559
3 1 0	7860
3 2 1	7365

The $\bar{B}$ value found from the double-axis diffraction is $3{\cdot}08 \pm 0{\cdot}43$ Å^2 which corresponds to the Debye temperature (θ) of 97 ± 7 K. $\bar{B}$ from the triple-axis diffraction mode is $3{\cdot}07 \pm 0{\cdot}22$ Å^2 corresponding to the Debye temperature of $97 \pm 3{\cdot}5$ K. The values are compared in Table 1 with the $\bar{B}$ values obtained by other workers.

The present $\bar{B}$ values are in excellent agreement with the mass-weighted average of the parameters B_{Tl} and B_{Cl} measured by X-ray diffraction by Haav, Peljo & Sourtti (1977). It is clear that in addition to giving experimental support to the earlier measurements, there is no discrepancy between the X-ray and neutron diffraction $\bar{B}$ values for TlCl.

The Debye temperature being low, it would be interesting to make studies on the anharmonic aspects of the atomic vibrations in this substance by measuring $\bar{B}$ as a function of temperature. Large anharmonic effects are expected in such measurements.

References

AHMED, N., BEG, M. M., BUTT, N. M., KHAN, Q. H. & ASLAM, J. (1977). *J. Nucl. Mater.* **68**, 365–366.

BATS, J. W. (1976). PhD Thesis, pp. 47–49. Twente Univ. of Tech., The Netherlands.

BEG, M. M. (1976). *Acta Cryst.* A**32**, 154–156.

BEG, M. M., ASLAM, J., BUTT, N. M., KHAN, Q. H. & ROLANDSON, S. (1974). *Acta Cryst.* A**30**, 662–667.

BUTT, N. M., AHMED, N., BEG, M. M., ATTA, M. A., ASLAM, J. & KHAN, Q. H. (1976). *Acta Cryst.* A**32**, 674–675.

CAGLIOTI, G. (1964). *Acta Cryst.* **17**, 1202–1213.

CHIPMAN, D. R. & PASKIN, A. (1959). *J. Appl. Phys.* **30**, 1998–2001.

GLUYAS, M., HUNTER, R. & JAMES, B. W. (1975). *J. Phys. C*, **8**, 271–282.

GROENEWEGEN, P. P. M. & HUISZOON, C. (1972). *Acta Cryst.* A**28**, 166–169.

HAAV, A. A., PELJO, E. & SOURTTI, P. (1977). *Phys. Status Solidi B*, **80**, 255–264.

JEX, H., MÜLLNER, M. & DYCK, W. (1974). *Phys. Status Solidi B*, **61**, 241–246.

JOSHI, S. K. & MITRA, S. S. (1960). *Proc. Phys. Soc.* **76**, 295–298.

KORHONEN, U. & LINKOAHO, M. (1966). *Ann. Acad. Sci. Fenn. Ser. A*6, No. 195, pp. 1–12.

MYUIRSEPP, T. K. & KHAAV, A. A. (1976). *Sov. Phys. Crystallogr.* **21**, 465–466.

RACCAH, P. M. & ARNOTT, R. J. (1967). *Phys. Rev.* **153**, 1028–1031.

SANGER, P. L. (1969). *Acta Cryst.* A**25**, 694–702.

SOURTTI, P. (1967). *Ann. Acad. Sci. Fenn. Ser. A*6, No. 240, pp. 1–33.

WILLIS, B. T. M. & PRYOR, A. (1975). *Thermal Vibrations in Crystallography*, pp. 121–122. Cambridge Univ. Press.