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X-ray determination of Debye–Waller factors of NaBr and NaI

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Abstract

The Debye–Waller factors of NaBr and NaI have been determined from X-ray diffraction intensities measured at room temperature with a powder X-ray diffractometer. The resulting values are: $B^+ = 1.55$ (15) and $B^- = 1.14$ (10) Å² for NaBr and $B^+ = 2.63$ (20) and $B^- = 1.81$ (15) Å² for NaI.

1. Introduction

A recent compilation of the Debye–Waller factors of cubic compounds by Butt *et al.* (1993) indicates that among the sodium halides there are as many as ten reports on the Debye–Waller factors of NaCl, four on NaF and none on NaBr and NaI. The purpose of this communication is to report the results of an experimental determination of the Debye–Waller factors of NaBr and NaI.

2. Experimental

Integrated intensities were measured using a Jeol JDX-8P powder X-ray diffractometer fitted with an NaI(Tl) scintillation counter. Filtered Cu radiation was employed. As both materials are hygroscopic, they were first heated to 470 K in a crucible and then transferred to an agate and mortar kept on a hot plate. After grinding on the hot plate, the powder was quickly transferred to the sample holder and covered with scotch tape. The effective absorption correction for such a sample is angle independent and is merged into the scale factor. The experimental conditions were so chosen that errors due to surface roughness, porosity, extinction and preferred orientation are minimized. The measured intensities are corrected for temperature diffuse scattering by the method suggested by Chipman & Paskin (1959). The application of the TDS correction increases the values of the B factors by about 2%. This is in agreement with the observation of Merisalo & Paakkari (1967) in the case of NaCl. All measurements were made at room temperature [295 (3) K].

The Debye–Waller factors pertaining to the two ions (B^+ and B^-) were determined from the intensities of the all-even and all-odd reflections by the method first used by Waller & James (1927), discussed in detail by James (1967) and followed by several workers (Wasastjerna, 1946; Houska, 1964; Atoji, 1972; Krivy & Sedivy, 1973; Subhadra *et al.*, 1992).

3. Discussion

The experimental values of the Debye–Waller factors of NaBr and NaI are given in Table 1. The Debye–Waller factors of NaBr and NaI have been calculated theoretically by (a) Gupta (1975) using an 11-parameter shell model and (b) Kushwaha

Table 1. *Experimental and theoretical values of the Debye–Waller factors B (Å²) of NaBr and NaI at room temperature*

Crystal	Experimental		Theoretical			
	B^+	B^-	Model (a) B^+	Model (a) B^-	Model (b) B^+	Model (b) B^-
NaBr	1.55 (15)	1.14 (10)	1.89	1.55	1.75	1.70
NaI	2.63 (25)	1.81 (15)	2.41	1.96	2.47	2.21

(1981) using a 7-parameter bond bending force model. These theoretical values at room temperature are also given in Table 1. A careful examination of the experimental and theoretical values given in Table 1 reveals the following features:

(i) It is generally observed that, in a given compound, the heavier (lighter) atom has the smaller (larger) amplitude of vibration and, hence, the smaller (larger) Debye–Waller factor (Menz, 1968; Linkoaho, 1969; Scheringer, 1973). This trend is also observed in the experimental as well as theoretical values of the Debye–Waller factors of NaBr and NaI.

(ii) The experimental and theoretical values of the Debye–Waller factors of both the ions show an increase as the Br ion is replaced by the I ion.

(iii) The experimental values of the Debye–Waller factors are of the same order as the theoretical values. The agreement between experimental and theoretical values is closer in the case of NaI than in the case of NaBr. However, the accuracy of about 10% in the present experimental results is not sufficient to differentiate between the values from the two models.

References

- Atoji, M. (1972). *Acta Cryst.* **A28**, 603.
 Butt, N. M., Bashir, J. & Nasir Khan, M. (1993). *Acta Cryst.* **A49**, 171–174.
 Chipman, D. R. & Paskin, A. (1959). *J. Appl. Phys.* **30**, 1998–2001.
 Gupta, R. K. (1975). *Phys. Rev. B*, **12**, 4452–4459.
 Houska, C. R. (1964). *J. Phys. Chem. Solids*, **25**, 359–365.
 James, R. W. (1967). *The Optical Principles of X-ray Diffraction*. London: Bell.
 Krivy, I. & Sedivy, J. (1973). *Phys. Status Solidi A*, **19**, 259–264.
 Kushwaha, M. S. (1981). *Nuovo Cim.* **65**, 285–292.
 Linkoaho, M. V. (1969). *Acta Cryst.* **A25**, 450–455.
 Menz, W. (1968). *Z. Phys.* **211**, 183–188.
 Merisalo, M. & Paakkari, T. (1967). *Acta Cryst.* **23**, 1107–1109.
 Scheringer, C. (1973). *Acta Cryst.* **A29**, 82–86.
 Subhadra, K. G., Raghavendra Rao, B. & Sirdeshmukh, D. B. (1992). *Pramana J. Phys.* **38**, 681–683.
 Waller, I. & James, R. W. (1927). *Proc. R. Soc. London Ser. A*, **117**, 214–223.
 Wasastjerna, J. A. (1946). *Soc. Sci. Fenn. Commun. Phys. Maths*, **13**, 1–24.