SHORT COMMUNICATIONS

ATOMIC VIBRATION AMPLITUDES FOR Pb AND S IN PbS

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THE mean Debye-Waller factor for PbS was first reported[1] using data on intensities of Bragg reflections recorded with a diffractometer fitted with a GM counter. These intensities were not corrected for the dead time effect of the counter and the data re-analysed[2] after a correction for dead time following a procedure suggested by Chipman[3]. As the main motivation for these experiments was the x-ray determination of the Debye temperature of PbS, only the mean Debye-Waller factor was determined and no attempt was made to evaluate the Debye-Waller factors of the individual atoms.

The Debye-Waller factors are related to the amplitude of atomic vibration ($B = 8\pi^2\mu^2/3$) and, in general, the amplitude of vibration of a heavier atom in a crystal will have a lower value than that for the lighter atom. Measurements by Keffer *et al*[4] of the Debye-Waller factors for PbTe revealed that the amplitude of vibration of the heavier Pb atom is larger than that of the lighter Te atom. This unusual observation was supported by lattice dynamical calculations[4] and also by independent experiments[5]. Recently, Kulkarni and Bichile[6] observed a similar effect in another lead salt, $Pb(NO_3)_2$. These observations generate an interest in the determination of the Debye-Waller factors of the individual atoms in PbS. The results of such a study are reported in this communication.

The integrated intensities of twelve x-ray Bragg reflections from a powder sample were measured with a powder diffractometer using filtered copper radiation. The intensities were corrected for thermal diffuse scattering and dead time effect. Atomic scattering factors for Pb were taken from Cromer and Waber[7] and those for S from International Tables for Crystallography[8]; the atomic scattering factors were corrected for anomalous dispersion[9].

The Debye-Waller factors were determined by combining the intensity data on the all-even and all-odd reflections following the method first employed by Waller and James[10] for sodium chloride and later used by several workers[11-14]. The working equations are given by Krivy and Sedivy[14].

The resulting values of the Debye-Waller factors are: $B_{Pb} = 1.36 \pm 0.10\,\text{Å}^2$ and $B_S = 0.78 \pm 0.03\,\text{Å}^2$. The corresponding values of the rms amplitude of vibration are: 0.228 ± 0.009 Å for Pb and 0.172 ± 0.004 Å for S. Thus, here again, as in the case of PbTe and $Pb(NO_3)_2$, the values of the Debye-Waller factor and the amplitude of vibration for the heavier lead atom are larger than those for the lighter partner-atom. Confirmation of the results by lattice dynamical calculation is desirable.

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