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Debye–Waller factors for magnesium oxide.

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The Debye–Waller factors for magnesium oxide have been calculated and compared with recent experimental results.

The Debye–Waller factors for MgO have been recently measured by Lawrence (1973) from X-ray diffraction. Earlier experimental measurements by Togawa (1965) on powder samples gave quite different values for the Debye–Waller factors. It was therefore decided at this stage to make a theoretical calculation of Debye–Waller factors in an attempt to resolve the paradox between the two sets of experimental data.

The Debye–Waller exponent, $W_\kappa(\mathbf{K})$ for all atoms κ in a cubic crystal may be written as (Buyers & Smith, 1968)

$$W_\kappa(\mathbf{K}) = B_\kappa \frac{\sin^2\theta}{\lambda^2}$$

with B_κ values independent of the magnitude of the momentum transfer **K**, which may be written as

$$B_\kappa = \frac{8\pi^2}{3} \sum_{\mathbf{q}j} \frac{\hbar}{NM_\kappa \omega_j(\mathbf{q})} [|e(\kappa|\mathbf{q}j)|^2 \{n[\omega_j(\mathbf{q})] + \tfrac{1}{2}\}] ,$$

where N is the number of unit cells in the crystal, $n[\omega_j(\mathbf{q})]$ is the population factor

$$[\exp(\hbar\omega_j(\mathbf{q})/K_\beta T) - 1]^{-1} ,$$

$e(\kappa|\mathbf{q}j)$ is the eigenvector of κth ion and $\omega_j(\mathbf{q})$ the eigen frequency for the jth branch corresponding to the wave vector **q**. 2θ is the scattering angle and λ is the wavelength of the radiation.

The eigen frequencies and corresponding eigenvectors for 8000 points in the Brillouin zone were computed using the shell-model parameters giving best fit to the neutron results. These are the parameters of Model B in paper of Sangster, Peckham & Saunderson, (1970). These eigen frequencies and eigenvectors were then used to calculate the B_κ values for magnesium and oxygen ions. The contribution from acoustic modes at the zone centre was taken into account by converting the summation into an integration over the volume 1/8000 of Brillouin zone along the lines of Buyers & Smith (1968) and assuming a Debye approximation over the volume of integration. This contribution was found to be less than 1% of the total value.

The calculated values at 300°K and experimental values are given in Table 1.

Table 1. *The B values for magnesium and oxygen ions*

	B(magnesium) in A$^{\circ 2}$	B(oxygen) in A$^{\circ 2}$
Theoretical values	0·30	0·33
Experimental values (Lawrence, 1973)	0·31 ± 0·01	0·34 ± 0·02
Experimental values (Togawa 1965)	0·24	0·19

Our theoretical values are in close agreement with the latest measurements of Lawrence (1973). Thus our calculations favour the recent measurements of Lawrence on a single-crystal specimen as against the measurement of Togawa on powder samples. The calculated results also show that the anharmonic contribution is negligibly small for this crystal at this temperature.

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Precession photography: an extrapolation method for more accurate cell dimensions.

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Shifts of reflexions caused by absorption of X-rays lead to systematic errors in cell dimensions. The effect is eliminated by an extrapolation procedure that affords an accuracy of about 0·1%. It can be used only if enough reciprocal rows are recorded.

One source of inaccuracy in cell dimensions is the shift of reflexions from their ideal positions caused by absorption of X-rays in the crystal. Although measurable in most photographs, the effect is best visible on reflexions with a blind spot in the centre: low-angle reflexions have a clear outline, higher-angle reflexions have a markedly stronger