LETTERS TO THE EDITOR

X-RAY DETERMINATION OF THE MEAN AMPLITUDE OF VIBRATION AND THE DEBYE TEMPERATURE OF Gd–Zn AND Gd–Mg

GADOLINIUM forms alloys with the cubic CsCl structure with cadmium, magnesium and zinc. There is, in general, a dearth of data regarding the lattice dynamical properties of these substances. The X-ray determination of the Debye temperature and mean amplitude of vibration of Gd–Mg and Gd–Zn has been carried out in these laboratories. The results are reported here.

In each case the material was reduced to a fine powder by grinding and a flat powder specimen was prepared. Measurements were made with a Philips PW 1051 diffractometer using CuKα radiation, filtered to eliminate Kβ radiation. An argon-filled G.M. counter was used to collect the intensity data. A 2θ scan was adopted.

The peak to background ratio of the reflections recorded was low for both Gd–Zn and Gd–Mg. Only seven measurable reflections in the case of Gd–Zn and six for Gd–Mg could be recorded in the angular range possible for the diffractometer.

The lattice constant of Gd–Zn was found to be 3·600 Å. This is in good agreement with the values 3·602 Å (Chao and Duwez[1]) and 3·601 Å (Buschow[2]) reported earlier. For Gd–Mg, Chao and Duwez report a value of 3·824 Å for the lattice constant, while Kripyakevich *et al.*[3] give a value 3·79 Å. The present value 3·812 Å is intermediate between the two. It must however be noted that the lattice constants were determined from the Bragg angles of the last three reflections recorded in each case and were not corrected for systematic errors.

The intensities were corrected for temperature diffuse scattering by the method of Chipman and Paskin[4], and for dead time effects by an approximate method proposed by Chipman[5], employing a value of 150 μs for the dead time of the counting apparatus.

For a flat powder specimen, the observed intensity I_0 is given by

$$I_0 = C\,(LP)\,J\,F_T^2 \qquad (1)$$

where C is a constant, LP the Lorentz-polarisation factor and J the multiplicity factor. Due to the small number of reflections recorded, a common Debye-Waller factor was assumed for both the atoms, in each of the crystals studied. With this approximation, the structure factor F_T for a CsCl type crystal is given by

$$F_T = Fe^{-B(\sin^2\theta/\lambda^2)} \qquad (2)$$

where θ is the Bragg angle, λ the wavelength of the radiation used and $F = f_A \pm f_B$. Here, f_A and f_B are the atomic scattering factors for atoms of type A and B. The plus sign refers to reflections with $(h + k + l)$ even and minus sign to reflections with $(h + k + l)$ odd.

The atomic scattering factors for Gd were taken from Cromer and Waber[6] and for Zn and Mg from those given in the *International Tables for X-ray Crystallography*[7] following a recommendation by Cromer[8]. The scattering factors were corrected for anomalous dispersion (Cromer and Liberman[9]).

The value of B can be obtained from a plot of log (I_0/I_c) against $\sin^2\theta/\lambda^2$, where $I_c = (LP)\,JF^2$. The root mean square amplitude of vibration $(\bar{u}^2)^{1/2}$ and the Debye temperature have been determined following the method described in an earlier paper[10].

Plots of log (I_0/I_c) against $\sin^2\theta/\lambda^2$ for both Gd–Zn and Gd–Mg are shown in Fig. 1. The values of the
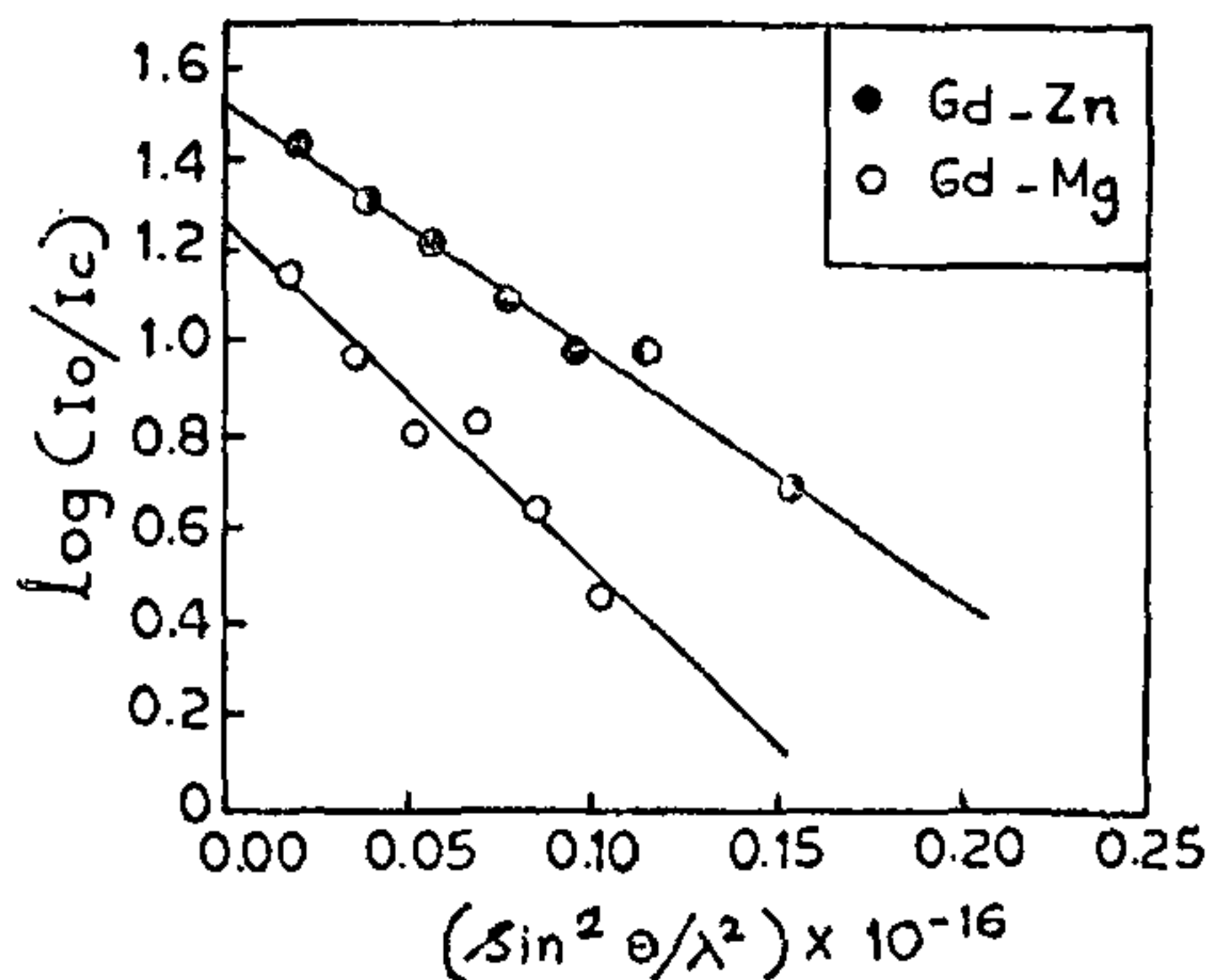
FIG. 1. Plot of log (I_0/I_c) and $\sin^2\theta/\lambda^2$ for Gd–Zn ($\bullet$) and Gd–Mg (O).

mean Debye-Waller factor B, the mean amplitude of vibration and the Debye temperature obtained are given in Table I.

There seems to be no earlier determination of the Debye temperature of either Gd–Zn or Gd–Mg by any method. The errors quoted refer only to random errors in the measurement of intensities.

From a consideration of other properties, Buschow[11] suggests that the two species of atoms exchange their sites to a certain degree. This is certain to affect the intensities. However, no information about this

aspect could be obtained due to the small number of reflections recorded.

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FRANCK-CONDON FACTORS AND r-CENTROIDS FOR THE $(A^2\Pi - X^2\Sigma^+)$ TRANSITION OF CN BY LANGER'S APPROXIMATION METHOD

THE Red band System of CN $(A^2\Pi - X^2\Sigma)$ transition is well known. Good deal of work, both experimental and theoretical, has been done on this particular system. In the present investigation we have chosen this transition for testing the validity of one of the less known methods of solving the Schrödinger wave equation approximately. This method is due to Langer[1], and very briefly it may be described as follows :

The one-dimensional Schrödinger wave equation is written as

$$\frac{d^2\psi}{dx^2} + \lambda^2 [E - V(x)]\psi = 0 \qquad (1)$$

where $\lambda^2 = 2\mu/\hbar^2$, $\mu =$ reduced mass, $\hbar =$ Planck's constant, $V(x) =$ Potential energy function.

The variable is changed from x to z through the relation

$$Z = x - x_e - \left(\frac{\sigma}{\lambda}\right) \qquad (2)$$

where

$$\sigma = -\frac{2V'''(x_e)\lambda E}{9[v''(x_e)]^2} \qquad (3)$$

$x_e =$ equilibrium internuclear distance; the primes indicate derivatives with respect to x. Equation (1) then becomes

$$\frac{d^2\psi}{dx^2} - [\lambda^2\psi_0{}^2(Z) + \lambda\psi_1(Z) + \psi_2(Z)]\psi = 0 \qquad (4)$$

where

$$\psi_0{}^2(Z) = V(z + x_e)$$

$$\psi_1(Z) = V(z + x_e)$$

$$\psi_2(Z) = \lambda^2 \left\{ V\left(z + x_e + \frac{\sigma}{\lambda}\right) - V(z - x_e) \right.$$
$$\left. - V'(z + x_e)\right\}.$$

Finally the solutions will come out as

$$\psi_n = \left[\frac{2V''(x_e)}{\pi}\right]^{1/4} \left(\frac{n!}{2^n}\right)^{1/2}$$

$$\times \frac{2(-1)^{(n-1)/2}}{\left(\frac{n-1}{2}\right)!} \frac{M_n\left[\frac{1}{2} + \frac{1}{4}, -\frac{1}{4}\right]}{\sqrt{\phi(z)}} \qquad (\xi)$$

where n is odd

$$\psi_n = \left[\frac{2V''(x_e)}{\pi}\right]^{1/4} \left(\frac{n!}{2^n}\right)^{1/2}$$

$$\times \frac{(-1)^{n/2}}{(n/2)!} \frac{M_n\left[\frac{1}{2} + \frac{1}{4}, -\frac{1}{4}\right]}{\sqrt{\phi(z)}} \qquad (\xi)$$

where n is even.

where the M's are confluent hypergeometric functions.

Using these wave functions and the Rydberg potential defined by

$$V(x) = -D[1 + a(x - x_e)]e^{-a(x-x_e)}$$