Acta Cryst. (1980). B**36**, 2857

On the atomic vibrations in the magnesium difluoride crystal. By GENEVIÈVE VIDAL-VALAT, *Laboratoire d'Infra-rouge, Groupe de Dynamique des Phases Condensées (LA 233), USTL, place Eugène Bataillon,* 34060 *Montpellier CEDEX, France,* JEAN-PIERRE VIDAL, *Laboratoire de Minéralogie Cristallographie, Groupe de Dynamique des Phases Condensées (LA 233), USTL, place Eugène Bataillon,* 34060 *Montpellier CEDEX, France,* CLAUDE M. E. ZEYEN, *Institut Laue–Langevin,* 156 *X Centre de Tri,* 38042 *Grenoble CEDEX, France* and KAARLE KURKI-SUONIO, *Department of Physics, University of Helsinki, Siltavuorenpenger* 20 *D, SF*-00170 *Helsinki* 17, *Finland*

(*Received* 16 *June* 1980; *accepted* 22 *July* 1980)

Abstract

The observed anisotropic Debye–Waller factors of MgF_2 and the relation between different interpretations of them are discussed with reference to a comment by Pauling [*Acta Cryst.* (1980), B**36**, 761–762].

Pauling (1980) has commented on an inadequacy in the discussion of anisotropic Debye–Waller factors in our recent neutron diffraction study on MgF_2 (Vidal-Valat, Vidal, Zeyen & Kurki-Suonio, 1979). He points out that the large amplitude of fluorine at room temperature should not be described in terms of librations of linear F—Mg—F molecules, but rather as vibrations involving the least change in the length of the strongest bonds.

The essence of our interpretation is, however, in the population of the low-lying lattice vibrational optical mode. In addition, an attempt was made to give a concrete picture of the nature of the coupled atomic vibrations of this mode. According to normal-mode analysis of the MgF_2 crystal (*cf.* Almairac & Benoit, 1974; Matsumoto, Urabe & Kanamori, 1978), the vibrations occur in a sense which corresponds to simultaneous librations of all Mg-centred F-octahedra. The description given by Pauling (1980) certainly gives a deeper insight into the physical cause for the low energy of this kind of mode.

Further, it should be noted that averaging of the amplitudes obtained in different refinements is not quite justified, because some of the extinction models used are clearly to be rejected. The extinction is concluded to be of mosaic-spread type and essentially isotropic. Consequently, the numerical values of mean-square amplitudes U_z, $U_{\parallel}$, $U_{\perp}$ to be referred to should be taken from the first column of our Table 9: at 52 K, 20, 26, 20 for Mg and 30, 36, 46 for F; and at 300 K, 36, 49, 57 for Mg and 62, 53, 121 for F, in units of 10^{-4} Å^2, rather than those given by Pauling (1980).

According to a subsequent investigation (Vidal, Vidal-Valat, Galtier & Kurki-Suonio, 1980) those values are further supported by lattice dynamical calculations and X-ray diffraction. The charge-density analysis indicates absence of any bonding charge density between nearest neighbours and, thus, strongly ionic nature of the bonding. This makes it still more obvious that – as emphasized by Pauling – one should not speak about molecules in MgF_2.

References

ALMAIRAC, R. & BENOIT, C. (1974). *J. Phys. C.* **7**, 2614–2648.

MATSUMOTO, M., URABE, K. & KANAMORI, H. (1978). *Indian J. Pure Appl. Phys.* **16**, 263–267.

PAULING, L. (1980). *Acta Cryst.* B**36**, 761–762.

VIDAL, J.-P., VIDAL-VALAT, G., GALTIER, H. & KURKI-SUONIO, K. (1980). In preparation.

VIDAL-VALAT, G., VIDAL, J.-P., ZEYEN, C. M. E. & KURKI-SUONIO, K. (1979). *Acta Cryst.* B**35**, 1584–1590.

0567-7408/80/112857-01$01.00