

The superscript a attached to both the M_{ij} and f_{ij} terms will refer to changes in these quantities due to the homogeneous deformation of each sublattice for zero inner displacements of the ions while under static strain. To get the f_{ij} , one must insert Eqs. (20) above into HM Eqs. (4.11). Then

$$\begin{aligned} f_{11} &= f_{11}^a = 2Ar_0^4 + 6Br_0^2 = 2r_0 v'''(r_0) \\ f_{12} &= f_{44} = f_{12}^a = f_{44}^a = 2Br_0^2 = 2v''(r_0) - 2v'(r_0)/r_0. \end{aligned} \quad (22)$$

e_T^* is related to the Szigeti effective charge e_S^* by:^{†20}

$$e_T^* = \left\{ \frac{\epsilon_\infty + 2}{3} \right\} e_S^*. \quad (23)$$

HM [Eq. (4.26a)] prescribe e_S^* via:

$$e_S^* = e_q^* + 2[m'(r_0) + 2m(r_0)/r_0] \quad (24)$$

where e_q^* is the electronic charge in coulombs.[‡] Substituting Eqs. (21) through (24) into (18), there results for the RS-structure:

[†]This equation holds for ZB-type crystals also.

[‡]Throughout this report we will employ the convention that quantities represented by an e and bearing an asterisk superscript are given in coulombs; whereas those bearing no asterisk superscript are dimensionless, being expressed in relation to the electronic charge. Thus, for example, $e_S = e_S^*/e_q^*$.

20. Maradudin, A.A., Montroll, E.W., Weiss, G.H., and Ipatova, I.P. (1971) "Theory of Lattice Dynamics in the Harmonic Approximation", Academic Press, New York.

$$A_{11} = -(\epsilon_0 - \epsilon_\infty)[1 - 4r_0 m''(r_0)/e_S^*]$$

$$A_{12} = -(\epsilon_0 - \epsilon_\infty)[1 - 4m'(r_0)/e_S^* + 4m(r_0)/r_0 e_S^*]$$

$$A_{44} = 4(\epsilon_0 - \epsilon_\infty)[m'(r_0) - m(r_0)/r_0]/e_S^* \quad (25)$$

$$B_{11} = -2R(\epsilon_0 - \epsilon_\infty) r_0 v'''(r_0)/\mu \omega_T^2$$

$$B_{12} = B_{44} = -2R(\epsilon_0 - \epsilon_\infty)[v''(r_0) - v'(r_0)/r_0]/\mu \omega_T^2$$

3.3.2 GENERAL EQUATIONS FOR ZINC BLENDE STRUCTURE

For crystals of the ZB-structure the elements of the M and f tensors are the sums of two contributions. The superscript a will denote the same meaning as stated in the previous section, while the superscript b will refer to changes in quantities due to the strain-induced inner displacements of the sublattices. Explicitly, Eqs. (4.61) and (4.67) of HM yield:

$$M_{11} = M_{11}^a + M_{11}^b = \frac{4}{9} Mr_0^4 + 4Nr_0^2$$

$$M_{12} = M_{12}^a + M_{12}^b = \frac{4}{9} Mr_0^4 + \frac{4}{3} Nr_0^2 \quad (26)$$

$$M_{44} = M_{44}^a + M_{44}^b = \left[\frac{4}{9} Mr_0^4 + \frac{4}{3} Nr_0^2 \right] + \left[\frac{R G \bar{m}}{\mu \omega_T^2} \right],$$

in which M_{11}^b and M_{12}^b turn out to be identically zero, μ and ω_T are expressed in gms and cm^{-1} , respectively, as usual, while the parameters G (in erg/cm) and $\bar{m}$ (in coul/cm) are given by HM [Eq. (4.46) and (4.68), respectively] as: