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Relation between Poisson's ratio and ionicity in simple binary cubic compounds

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Abstract

The nature of the atomic forces in solids may be obtained from a knowledge of the elastic constants. Covalent compounds have a tetrahedral structure, whereas ionic compounds have a rock salt or caesium chloride structure, and it is necessary that appropriate models should be applied to explain the elastic properties of covalent and ionic crystals because of the difference in the crystal symmetry and bonding character. Elastic properties of covalent and ionic compounds have been explained using a valence-force-field model and deformation dipole model respectively. A more qualitative interpretation concerning the relation between Poisson's ratio and ionicity in simple binary cubic compounds is given in this study.

1. Introduction

Elastic constants provide information on the nature of the atomic forces in solids. Poisson's ratio (ν) gives more information on the character of the bonding forces than any other elastic coefficient [1]. The so-called Cauchy relation [2] can be correlated with Poisson's ratio and the rariconstant theory [1] gives a basis of the Cauchy relation which depends on the following conditions: (1) the exclusive presence of central forces; (2) a centre of symmetry at every lattice site; (3) the disappearance of initial stresses. If these conditions are truly satisfied, elastic constants will be totally symmetric in their four subscripts, namely $C_{ijkl}=C_{ikjl}=C_{iljk}$, and Poisson's ratio is equal to 0.25. Compounds of the face-centred and body-centred cubic structures have an inversion centre of symmetry, whereas compounds of the diamond, zinc blende and wurtzite structures do not [3]. Consequently, the fulfilment of the Cauchy relation for the former structures offers a basis for the nature of the force field, whereas this is not so for the latter. The better the satisfaction of the Cauchy relation, the greater the preponderance of electrostatic forces and the more ionic the compound [4].

The ionicity scales of Pauling [5] and Phillips [6] are useful parameters in the analysis of experimental data relating to charge distributions. One of the practical applications of the concept of ionicity is in the development of interatomic potentials [7]. The ionicity (f_i) is not a direct measure of the ionic interaction energy, but rather a measure of the dipole moment [8]. It has a close relation with the structural stabilities of crystals and there is a critical value of ionicity around 0.785 which divides two stable, fourfold and sixfold structures [9–11]. Therefore covalent crystals have a tetrahedral structure, whereas ionic crystals have a rock salt or caesium chloride structure, and it is necessary that appropriate models should be applied to explain the elastic properties of covalent and ionic crystals because of the difference in the crystal symmetry and bonding character. They are cubic and their elastic behaviour can be expressed by only C_{11}, C_{12} and C_{44}.

The most useful phenomenological description of the interatomic interaction in the tetrahedrally coordinated crystal is the valence-force-field (VFF) model of Keating [12] and Martin [13]. All interatomic forces of the VFF model consist of bond-stretching (central force constant, α) and bond-bending (non-central force constant, β) terms. To compensate for the instability of open covalent crystals in terms of the shear deformation [14], Phillips [15, 16] introduced the bond charge model. The bond charge has a close relation with the non-central force constant which describes the crystal stability in response to the shear deformation [17]. Martin [13, 18] showed that the strong bond-bending term produced high values of shear moduli and they decreased markedly with an increase in ionicity in covalent crystals.

Several review articles [19, 20] have shown that the deformation dipole model (DDM) is one of the most widely used to study the lattice dynamics of binary

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solids, especially ionic compounds. Dipole moments in the DDM arise from the displacement of an ion as a rigid point charge and the redistribution of electronic charge in the overlapped region between nearest neighbour ions [21–24]; therefore, the interactions between two nearest neighbours are associated with the dipole moments which exist at the centre of each ion. However, the DDM failed to explain the Cauchy violation because of many-body interactions, of which the three-body components are most significant [25]. Consideration of these three-body interactions (TBI) is essential in predicting the cohesive energies and Cauchy violation in ionic crystals [26, 27]. The violation of the Cauchy relation has been explained through the effect of the angle bending force (ABF) in the framework of the DDM [28, 29].

Poisson's ratio can be expressed with the elastic coefficients (C_{11}, C_{12}, C_{44}) of cubic single crystals [1] or with elastic shear and bulk constants (G, B) of polycrystals [30]. These elastic constants are closely related to the ionicity [13, 18] and many researchers [31–33] have found a schematic relation between the elastic constants and ionicities for various covalent compounds. Consequently, we wish to report a correlation between Poisson's ratio and the ionicity of various compounds [34, 35]. It was found that Poisson's ratio increases with ionicity (decreases with covalency) for covalent crystals, but this behaviour is not automatically extended to strongly ionic compounds of rock salt and CsCl structures. However, in the previous article [35], a theoretical analysis was not fully made. In this study, we explore why different behaviour exists for the two groups of solids. For covalent compounds, the trend is explained through the non-central force constant which describes the structural stability against the shear deformation [12–18] and, for ionic compounds, the trend is explained through the use of the ABF constant in the framework of the DDM [26–29].

2. Calculation of Poisson's ratio and ionicity

In determining Poisson's ratio a distinction must be made between direct and indirect methods and between static and dynamic methods [1]. As it is rather difficult to measure Poisson's ratio, it is usually calculated indirectly from measured elastic constants of single crystals. Thus, the determination of any two values of Young's modulus, shear modulus or bulk modulus gives an indirect value of Poisson's ratio. The computing of these three elastic constants of polycrystals, with or without preferred orientations, from single-crystal data by suitable averaging is difficult. However, under the assumption of uniform strain, Voigt [36] averaged elastic coefficients which were dependent only on the values of the symmetrical combinations of the directional cosines. With the combination of bulk modulus and Voigt's shear modulus, which represented averaged elastic coefficients, we calculated indirect values of Poisson's ratio. This combination yielded fewer errors than any other method in the determination of Poisson's ratio [1, 37]. Hill [38] showed that Voigt's average gave a least upper bound, and Reuss' average [39], under the assumption of uniform stress, produced a greatest lower bound for Poisson's ratio. For comparison, they also represent average values at room temperature and 1 atm pressure.

The use of the concept of ionicity has taken several distinct forms in quantitative studies of solid state physics, *e.g.* a description of charge distribution of bonding, a spectroscopic classification of perfect solids and a framework for quantitative modelling of defects in polar solids [7]. To isolate trends associated entirely with ionicity, homologous systems, A^NB^{8-N} compounds, in which the hybridization states vary as little as possible should ideally be selected [6, 40]. A^NB^{8-N} crystal systems contain no complexities associated with d-shell electrons, have fully saturated bonding and have therefore been most widely studied experimentally as well as theoretically [41, 42]. There are two well-known definitions of ionicity. In the thermochemical approach of Pauling [5], the ionicity of the chemical bond is determined only by extra ionic energies, covalent energies not being used. In the dispersion theory of Phillips [6] and Van Vechten [43], the ionicity is determined through consideration of the ionic energy and covalent energy symmetrically. Due to the asymmetrical treatment of Pauling [5], there is less accuracy in his ionicity scale than in those of Phillips [6] and Van Vechten [43]. We used the ionicity values of Phillips [6] for most A^NB^{8-N} crystals, except for some compounds whose ionicity values were not given. CdTe, GaP, ZnSe and ZnTe were taken from Van Vechten [44], Hg-containing compounds from Kumazaki [31], ZnO from Lawaetz [45] and CsCl compounds from Levine [46]. Some binary compounds which have more than eight valence electrons, but maintain a cubic zinc blende, rock salt or CsCl structure are included as follows: CoO and MnO from Levine [47] and TlBr and TlCl from Lucovsky *et al.* [48].

3. Results and discussion

Two distinct differences between fourfold and sixfold or eightfold compounds were mentioned earlier. Firstly, there is a lack of an inversion centre of symmetry for fourfold compounds, which nullifies the physical meaning of the fulfilment of the Cauchy relation. Secondly, the directed sp^3-hybridized bonding contributes to the structural stability of fourfold crystals, whereas electrostatic interactions contribute to the structural stability of sixfold and eightfold compounds. As a result it seems plausible to analyse these two groups of compounds with the application of appropriate models to enhance the accuracy of physical trends.

3.1. *Fourfold compounds*

The VFF model of Keating [12] and Martin [13] has virtues of rotational invariance because all distortions are described by the bond length (r) and angle (θ). This model uses a reduced modulus to remove the dependence of the bond length. The reduced modulus, C_{ij}^*, is normalized as follows: $C_{ij}^* = C_{ij}/C_0$ where $C_0 = e^2/r^4$ and e is the electronic charge. Therefore, reduced moduli have a direct relation to the bonding character of compounds [13]. In addition to the compounds handled in Martin's work [13, 18], we obtained moduli of cuprous and silver halides and mercury chalcogenides which are characterized by a close d-shell cation. In the VFF model, the reduced shear modulus C_s^*, which is equal to $(C_{11}^* - C_{12}^*)/2$, is related to the non-central bond-bending term (β) and the coulombic contribution. However, the reduced shear modulus C_{44}^* is related to the central bond-stretching term (α) and internal strain as well as β and the coulombic contribution. Lucovsky *et al.* [48] have suggested a reduced bond-bending force constant β^* so that dipole interaction contributions are required to the elastic constants. β^* is described by squared e_l^*, the localized effective charge, instead of the effective charge parameter used by Martin [13] in the following way: $\beta^* = 2C_s^* - 0.052e_l^{*2}$. In long-wave acoustic modes, Weber [49] has also shown that the strong bond–bond coupling is essential for the stability of the diamond structure against shear deformation, and therefore it is reasonable to explain the structural stability of covalent compounds against shear through the β^* term alone. We obtained the value of β^*, which is considered as a measure of shear stability, and the result is given in Table 1 together with other calculated parameters.

The reduced shear modulus C_s^* decreases more systematically than C_{44}^* with an increase in ionicity as shown in Fig. 1. Pure covalent elements included in the figure are C, Si and Ge. Figure 2 shows that the reduced bond-bending force constant β^* decreases systematically as the ionicity increases and approaches zero near the critical ionicity beyond which the fourfold structure is no longer stable. This trend is different from Martin's work [13] to some extent. He suggested the ratio of β/α as a limit of shear stability. Moreover, he proposed that the ratio would tend to approach zero in the ionic limit where the ionicity is equal to unity. However, Hg compounds [31], cuprous halides [32] and AgI [33] show very low values of the ratio

TABLE 1. Compilation of several parameters (C_s^*, C_{44}^*, β^*, γ, ν and f_i) of fourfold covalent compounds

Compound	C_s^*	C_{44}^*	γ	ν	β^*	f_i
AgI[a]	0.044	0.221	0.154	0.393[b]	0.000	0.770[h]
AlSb	0.487	0.899	0.382	0.260[c]	0.889	0.426[h]
BeO	0.370	0.640	0.493	0.204[d]	0.544	0.602[h]
CdS[a]	0.220	0.430	0.212	0.356[d]	0.246	0.685[h]
CdSe[a]	0.200	0.470	0.215	0.354[d]	0.222	0.699[h]
CdTe[a]	0.225	0.535	0.240	0.339[c]	0.288	0.717[i]
CuBr[a]	0.081	0.217	0.178	0.377[e]	0.063	0.735[h]
CuCl[a]	0.059	0.177	0.175	0.379[e]	0.000	0.746[h]
CuI[a]	0.145	0.366	0.260	0.328[e]	0.133	0.692[h]
GaAs	0.506	0.926	0.432	0.234[c]	0.926	0.310[h]
GaP	0.530	0.949	0.436	0.231[c]	0.956	0.327[i]
GaSb	0.514	0.923	0.421	0.239[c]	0.979	0.261[h]
β-HgS[a]	0.170	0.470	0.191	0.369[f]	[g]	0.790[f]
HgSe[a]	0.179	0.488	0.201	0.363[f]	[g]	0.680[f]
HgTe[a]	0.235	0.590	0.241	0.338[f]	0.256	0.650[f]
InP	0.403	0.832	0.336	0.284[c]	0.672	0.421[h]
InAs	0.385	0.801	0.361	0.271[c]	0.699	0.357[h]
InSb	0.406	0.811	0.346	0.279[c]	0.769	0.321[h]
SiC	0.650	1.370	0.601	0.153[d]	1.253	0.177[h]
ZnO[a]	0.300	0.360	0.236	0.342[d]	0.381	0.660[j]
ZnS[a]	0.255	0.603	0.304	0.302[c]	0.333	0.623[h]
ZnSe[a]	0.253	0.694	0.368	0.267[c]	0.358	0.630[i]
ZnTe[a]	0.321	0.655	0.325	0.290[c]	0.484	0.609[i]

[a] Closed d-shell compound.
[b] Ref. 33.
[c] Ref. 13.
[d] Ref. 18.
[e] Ref. 32.
[f] Ref. 31.
[g] Due to unknown value of e_l^*.
[h] Ref. 6.
[i] Ref. 44.
[j] Ref. 45.

References for C_s^*, C_{44}^*, γ and β^* are the same as for ν for each compound. $\beta^* = 2C_s^* - 0.052e_l^{*2}$, e_l^* from ref. 48.

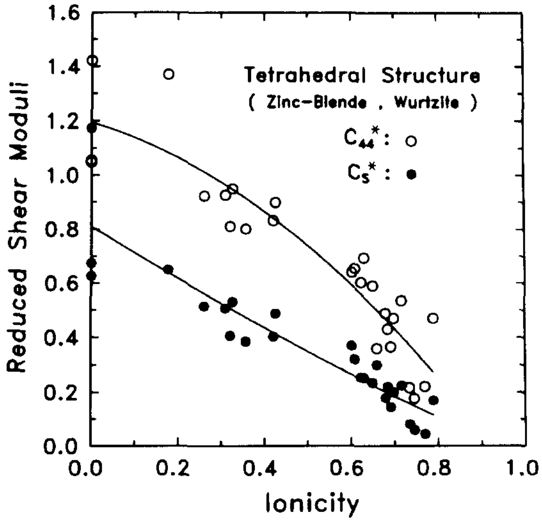

Fig. 1. Relation between reduced shear moduli (C_s^*, C_{44}^*) and ionicity of covalent compounds.

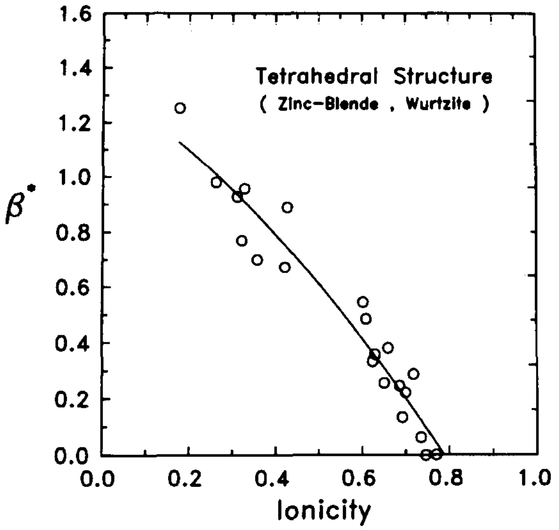

Fig. 2. Reduced bond-bending force constants (β^*) *vs.* ionicity of covalent compounds.

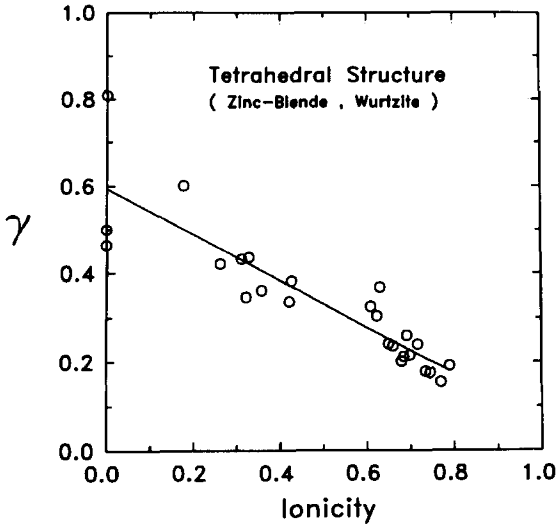

Fig. 3. Relation between γ ($=2G_v^*/3B^*$) term and ionicity of covalent compounds.

near the critical ionicity. Van Vechten [50] also showed that the VFF model of Keating and Martin seriously overestimated the bond-bending force constants for the compounds whose values of ionicity are greater than 0.5 and the β term goes to zero when the ionicity reaches its critical value rather than unity. Under the assumption of uniform strain, the reduced Voigt shear modulus (G_v^*) is expressed as follows: $G_v^* = 2C_s^*/5 + 3C_{44}^*/5$ [37]. It is quite natural to expect that G_v^* decreases strongly with an increase in ionicity from Fig. 1, whereas the reduced bulk modulus, $B^* = (C_{11}^* + 2C_{12}^*)/3$ decreases weakly with ionicity. Poisson's ratio can be expressed by the γ ($=2G_v^*/3B^*$) term in the following way: $\nu = (1-\gamma)/(2+\gamma)$, where the γ term decreases with an increase in ionicity up to the critical ionicity point of Fig. 3.

Consequently, Poisson's ratio should increase with ionicity regardless of the relative magnitude between C_{12}^* and C_{44}^* as shown in Fig. 4. Compounds near the critical ionicity have larger values of Poisson's ratio than others in the same class. These trends are clearly dependent on the values of β^* which describe the structural stability against the shear deformation. The trends of the elastic constants of compounds characterized by a closed d-shell cation will be analysed with the application of TBI [51] in the next section.

3.2. Sixfold and eightfold compounds

As mentioned earlier, the dipole moments in the DDM change the shear deformations, cause multiple interactions, affect the elastic constants and thus lead to the violation of the Cauchy relation. Cauchy relation violation in diatomic cubic crystals has been explained by including the effect of the ABF in the framework of the DDM [28, 29]. The ABF constant (C) in the long-wave acoustic mode is defined as follows: $C = C_{12}^* - C_{44}^*$. The interaction mechanisms [52] beyond the dipole approximation are due mainly to charge transfer and shell breathing which are manifested as TBI [25–27]. Short-range TBI [51, 53–56] and long-range TBI are both important. Consideration of the following three interactions (in addition to the two-body interaction of the nearest neighbours) is essential to explain the elastic properties of ionic solids [57]: TBI, next nearest neighbour interaction and van der Waals' interaction.

With this in mind, we obtained the reduced shear moduli C_{12}^* and C_{44}^* at room temperature and 1 atm pressure for 16 alkali halide crystals (Table 2). Cauchy relation violation occurs in Fig. 5 to some extent, in spite of the expectation that alkali halides with a rock

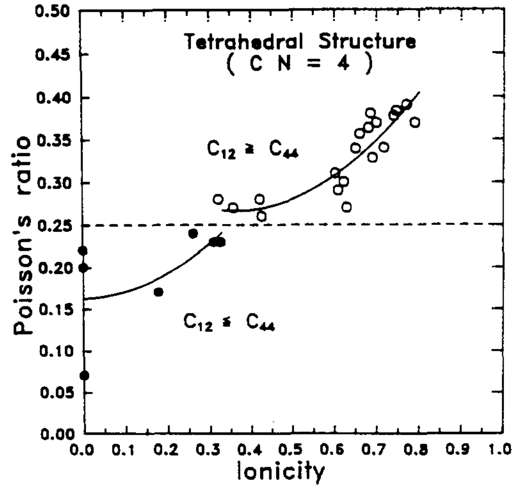

Fig. 4. Poisson's ratio *vs.* ionicity of compounds with a coordination number of four. Filled symbols are for $C_{12} \leq C_{44}$ and open symbols vice versa (adapted from ref. 35).

TABLE 2. Compilation of several parameters (C_{11}*, C_{12}*, C_{44}*, ν and f_i) of sixfold and eightfold compounds (from ref. 37)

Compound	C_{11}*	C_{12}*	C_{44}*	ν	f_i
AgBr[a]	1.696	0.994	0.217	0.397	0.850[b]
AgCl[a]	1.541	0.928	0.160	0.409	0.856[b]
CaO	3.136	0.848	1.165	0.210	0.913[b]
KBr	1.769	0.277	0.261	0.254	0.952[b]
KCl	1.845	0.322	0.339	0.246	0.953[b]
KF	1.428	0.314	0.282	0.260	0.955[b]
KI	1.819	0.302	0.244	0.265	0.950[b]
LiBr	0.980	0.468	0.475	0.248	0.899[b]
LiCl	0.934	0.427	0.469	0.235	0.903[b]
LiF	0.788	0.298	0.445	0.187	0.915[b]
LiI	1.004	0.493	0.475	0.256	0.890[b]
MgO	2.457	0.747	1.271	0.171	0.841[b]
NaBr	1.083	0.305	0.253	0.270	0.934[b]
NaCl	1.362	0.348	0.348	0.250	0.935[b]
NaF	1.220	0.305	0.352	0.236	0.946[b]
NaI	1.445	0.429	0.343	0.274	0.927[b]
RbBr	1.942	0.293	0.235	0.264	0.957[b]
RbCl	1.869	0.313	0.244	0.268	0.955[b]
RbF	1.562	0.342	0.249	0.276	0.960[b]
RbI	2.052	0.298	0.233	0.268	0.951[b]
SrO	2.890	0.785	1.065	0.212	0.926[b]
CoO	4.383	2.466	1.393	0.326	0.858[d]
MnO	3.799	2.044	1.346	0.308	0.887[d]
CsBr	2.459	0.639	0.620	0.253	0.965[c]
CsCl	2.580	0.621	0.566	0.259	0.962[c]
CsI	2.589	0.705	0.657	0.258	0.965[c]
TlBr	2.307	0.894	0.464	0.319	0.900[e]
TlCl	2.111	0.805	0.400	0.322	0.900[e]

[a] Closed d-shell compound.
[b] Ref. 6.
[c] Ref. 46.
[d] Ref. 47.
[e] Ref. 48.

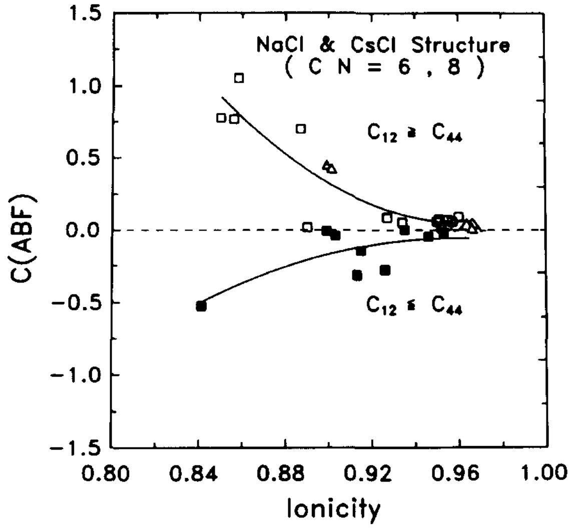

Fig. 5. Angle-bending force constant (*C*) *vs.* ionicity of ionic compounds with a coordination number of six or eight.

salt structure should satisfy the Cauchy relation. In TBI, the ABF term from a given shell is negative if the pair interaction is repulsive and it is positive if attractive [53–55]. The markedly large value of C_{44}* compared with C_{12}* of LiF in contrast with the other alkali halides results from the overlap between large negative ions, *i.e.* the very small central positive ion of LiF plays a key role resulting in the significant repulsive field. The ABF constants of most alkali halides have positive values, whereas LiF has a large negative value.

Owing to the high electrostatic compression in II–VI oxide compounds with a rock salt structure, their nearest neighbour distances are shorter and the electrostatic bonding stronger than alkali halides [54]; therefore, the pair interactions are repulsive and the ABF constants of these oxides are negative. MgO has a stronger repulsive field than the rest because of a smaller positive ion. Moreover, the van der Waals' interactions between the next nearest neighbours are weaker than those of alkali halides [58]. MgO has the largest negative ABF constant of these oxides. For CoO and MnO, C_{12}* is also larger than C_{44}*. Due to the large nearest neighbour distances of CsCl compounds compared with alkali halides which have a large positive ion, the interactions between the reference ion and the first few shells of ions are attractive, but further shells do not develop significant ion repulsions [54]. Therefore, the three caesium halides have values of C_{12}* slightly larger than C_{44}*, whereas the two thallium halides have much higher values of C_{12}* than C_{44}*.

Poisson's ratio is closely related to the ABF constant because its definition through Voigt's method for isotropic polycrystals is as follows

$$\nu = \frac{1-2G_v^*/3B^*}{2+2G_v^*/3B^*}$$

$$= \frac{1}{4} + \frac{5}{4}\,\frac{C_{12}^* - C_{44}^*}{(2C_{11}^* + 3C_{12}^* + C_{44}^*)} \qquad (1)$$

If the ABF is positive, Poisson's ratio is greater than 0.25 and vice versa. Moreover, the ABF should be reduced to zero with an increase in ionicity because ideally ionic central solids satisfy the Cauchy relation and the angle-bending forces should disappear at the ionic limit. For the case of $C_{12} \leqslant C_{44}$, the ABF is negative and its magnitude decreases slightly with ionicity to approach zero. However, for the compounds whose C_{12} value is greater than C_{44}, it is positive and should decrease with ionicity to disappear.

Poisson's ratios obtained in this way are shown in Fig. 6. The trend is quite similar to that of Fig. 5 as expected. There are some notable points. The value of Poisson's ratio of LiF is located well below 0.25 because of the large C_{44}*. Similarly, II–VI oxides have Poisson's ratios smaller than 0.25 because of the large

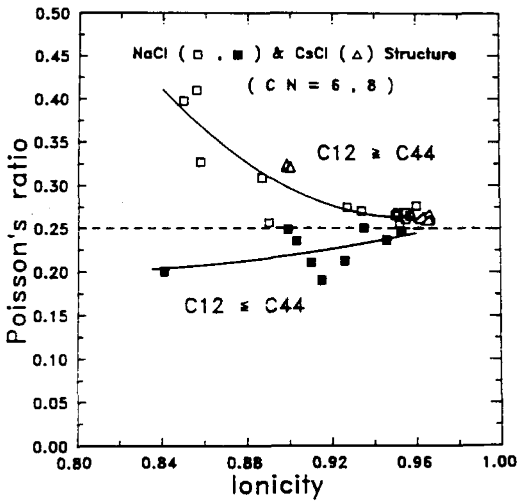

Fig. 6. Poisson's ratio *vs.* ionicity of compounds of NaCl structure (□, ■) and CsCl structure (△). Filled symbols are for $C_{12} \leqslant C_{44}$ and open symbols vice versa (adapted from ref. 35).

C_{44}* values, and they tend to approach 0.25 with increasing ionicity. In contrast, Poisson's ratios of CoO and MnO are larger than 0.25 because of higher values of C_{12}*. Caesium halides have Poisson's ratios near 0.25, whereas thallium halides have larger values.

4. Final discussion

There are some interesting features in copper, silver, zinc, cadmium and mercury compounds with a closed d-shell cation [51]. The elastic properties of these compounds can be analysed with the application of TBI. They have a complete outer shell of d electrons whose excited state lies considerably lower than that of an ion with a rare gas configuration. Therefore the cation–cation and cation–anion pairs interact attractively in a short range. Consequently, these interactions lead to a high value of C_{12}* compared with C_{44}* and the difference between the two constants should increase with ionicity up to the critical ionicity as shown in Fig. 7. This trend implies from eqn. (1) that the Poisson's ratios of these compounds are larger than 0.25 and should increase with ionicity. There is also a notable point in silver halides with an NaCl structure compared with most compounds with zinc blende or wurtzite structures, *i.e.* very strong two-body van der Waals' forces yield very large values of C_{12}* and three-body van der Waals' forces contribute mainly to the violation of the Cauchy relation [59].

The general relation between the Poisson's ratio and ionicity of ionic and covalent compounds seems to be very different. Poisson's ratios of covalent crystals increase with ionicity up to the critical ionicity regardless of the relative magnitude of C_{12} and C_{44}, whereas those of ionic compounds are directly dependent on the relative magnitude between C_{12} and C_{44}, which seems to be dependent on the ionicity.

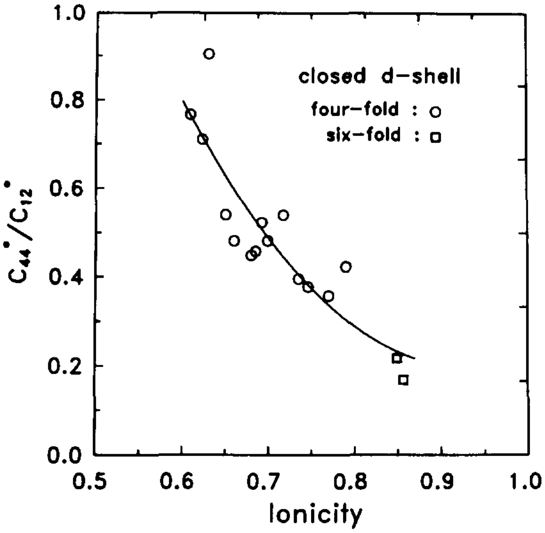

Fig. 7. Ratio of reduced shear moduli (C_{44}*/C_{12}*) *vs.* ionicity of closed d-shell compounds.

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References

1 W. Köster and H. Franz, *Metall. Rev., 6* (1961) 1.
2 H. B. Huntington, *The Elastic Constants of Crystals,* Academic Press, New York, 1958, p. 22.
3 M. J. P. Musgrave, *Crystal Acoustics,* Holden-Day, San Francisco, CA, 1970, p. 57.
4 B. G. Dick, Jr. and A. W. Overhauser, *Phys. Rev., 112* (1958) 90.
5 L. Pauling, *The Nature of the Chemical Bond,* Cornell University Press, Ithaca, NY, 3rd edn., 1960, p. 97.
6 J. C. Phillips, *Rev. Mod. Phys., 42* (1970) 317.
7 C. R. A. Catlow and A. M. Stoneham, *J. Phys. C, 16* (1983) 4321.
8 N. E. Christensen, S. Satpathy and Z. Pawlowska, *Phys. Rev. B, 36* (1987) 1032.
9 J. C. Phillips, *Phys. Rev. Lett., 27* (1971) 1197.
10 E. Louis and F. Flores, *Phys. Rev. B, 24* (1981) 4899.
11 J. R. Chelikowsky, *Phys. Rev. B, 34* (1986) 5295.
12 P. N. Keating, *Phys. Rev., 145* (1966) 637.
13 R. M. Martin, *Phys. Rev. B, 1* (1970) 4005.
14 R. M. Martin, *Phys. Rev., 186* (1969) 871.
15 J. C. Phillips, *Phys. Rev., 166* (1968) 832.
16 J. C. Phillips, *Phys. Rev., 168* (1968) 905.

17 A. P. Rusakov and M. V. Anfimov, *Phys. Status Solidi B, 75* (1976) 73.

18 R. M. Martin, *Phys. Rev. B, 6* (1972) 4546.

19 R. K. Singh, *Current Trend in Lattice Dynamics,* IPA, India, 1979, p. 137.

20 J. R. Hardy and A. M. Karo, *The Lattice Dynamics and Statics of Alkali Halide Crystals,* Plenum, New York, 1979, p. 1.

21 J. R. Hardy and A. M. Karo, *Philos. Mag., 5* (1960) 859.

22 J. R. Hardy, *Philos. Mag., 7* (1962) 315.

23 A. M. Karo and J. R. Hardy, *Phys. Rev., 129* (1963) 2024.

24 A. M. Karo and J. R. Hardy, *Phys. Rev., 181* (1969) 1272.

25 A. N. Basu, D. Roy and S. Sengupta, *Phys. Status Solidi A, 23* (1974) 11.

26 M. P. Verma and R. K. Singh, *Phys. Status Solidi B, 33* (1969) 769.

27 J. Andzelm and L. Piela, *J. Phys.· C, 10* (1977) 2269.

28 S. S. Jaswal and J. R. Hardy, *Phys. Rev., 171* (1968) 1090.

29 S. L. Cunningham, T. P. Sharma, S. S. Jaswal, M. Hass and J. R. Hardy, *Phys. Rev. B, 10* (1974) 3500.

30 H. M. Ledbetter, *J. Phys. Chem. Solids, 34* (1973) 721.

31 K. Kumazaki, *Phys. Status Solidi A, 33* (1976) 615.

32 R. C. Hanson, J. R. Hallberg and C. Schwab, *Appl. Phys. Lett., 21* (1972) 490.

33 T. A. Fjeldly and R. C. Hanson, *Phys. Rev. B, 10* (1974) 3569.

34 H. M. Lee and W.-J. Lee, *Scr. Metall. Mater., 25* (1991) 965.

35 J. W. Soh and H. M. Lee, *Scr. Metall. Mater., 27* (1992) 783.

36 W. Voigt, *Lehrbuch der Krystallphysik,* Teubner, Leipzig, 1928, p. 962.

37 G. Simmons and H. Wang, *A Handbook of Single Crystal Elastic Constants and Calculated Aggregate Properties,* MIT Press, 2nd edn., 1971.

38 R. Hill, *Proc. Phys. Soc. London (A), 65* (1952) 349.

39 A. Reuss, *Z. Angew. Math. Mech., 9* (1929) 49.

40 J. K. Burdett, G. D. Price and S. L. Price, *Phys. Rev. B, 24* (1981) 2903.

41 J. C. Phillips, *Bonds and Bands in Semiconductors,* Academic Press, New York, 1973, p. 27.

42 W. A. Harrison, *Electronic Structure and the Properties of Solids,* Freeman, San Francisco, CA, 1980, p. 38.

43 J. A. Van Vechten, *Phys. Rev., 182* (1969) 891.

44 J. A. Van Vechten, *Phys. Rev. B, 3* (1971) 562.

45 P. Lawaetz, *Phys. Rev. B, 5* (1972) 4039.

46 B. F. Levine, *J. Chem. Phys., 59* (1973) 1463.

47 B. F. Levine, *Phys. Rev. B, 7* (1973) 2591.

48 G. Lucovsky, R. M. Martin and E. Burstein, *Phys. Rev. B, 4* (1971) 1367.

49 W. Weber, *Phys. Rev. B, 15* (1977) 4789.

50 J. A. Van Vechten, *Phys. Rev. B, 10* (1974) 4222.

51 E. Lombard, L. Jansen and R. Ritter, *Phys. Rev., 185* (1969) 1158.

52 A. N. Basu and S. Sengupta, *Phys. Status Solidi B, 29* (1968) 367.

53 E. Lombard and L. Jansen, *Phys. Rev., 136* (1964) A1011.

54 E. Lombard and L. Jansen, *Phys. Rev., 140* (1965) A275.

55 E. Lombard and L. Jansen, *Phys. Rev., 185* (1969) 1150.

56 A. K. Sarkar and S. Sengupta, *Phys. Status Solidi B, 58* (1973) 775.

57 J. Shanker, V. C. Jain and J. P. Singh, *Phys. Rev. B, 22* (1980) 1083.

58 M. J. L. Sangster, *J. Phys. Chem. Solids, 34* (1973) 355.

59 M. Bucher, *Phys. Rev. B, 30* (1984) 947.