Analytic relation between bulk moduli and lattice constants

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An analytic relation between the bulk modulus of a solid and its equilibrium lattice constant is sought by examining how the various components of the total structural energy scale with distance. Simple formulas are obtained for the bulk modulus and its pressure derivative. A comparison is made with an empirical scaling approach for diamond and zinc-blende materials.

I. INTRODUCTION

A simple formula for the bulk moduli of diamond and zinc-blende solids was obtained by one of us[1] using scaling arguments for the relevant energy and volume. It was argued that the dominant effect in these materials is the degree of covalency characterized by the Phillips homopolar gap[2] E_h and the volume of the bond charge, $\pi(2a_B)^2 d$, where d is the nearest-neighbor distance. Using the empirical relation[1,2] $E_h \propto d^{-2.5}$, the resulting formula for the bulk modulus is

$$B_0 = (1971 - 220\lambda)d^{-3.5} , \qquad (1)$$

where λ is an empirical parameter which accounts for the effect of ionicity; $\lambda = 0, 1, 2$ for group-IV, III-V, and II-VI semiconductors respectively. The units are GPa and Å for B_0 and d in Eq. (1). The accuracy of the above formula in predicting the bulk modulus is remarkably good with only a few percent error for most of the materials examined.[1]

In this paper, we explore the microscopic origin of the simple relation between the bulk modulus and nearest-neighbor distance. Starting with the pseudopotential total-energy formalism, we examine how the various energy components of the total energy scale with the lattice constant or Wigner-Seitz radius. From the total energy, an analytic expression for the bulk modulus is derived. The expression is different in structure from the empirical formula but gives similar numerical results. We also obtain an analytic expression for the pressure derivative of the bulk modulus, B_0'.

II. THE BULK MODULUS
AND ITS PRESSURE DERIVATIVE

Within the local-density formalism[3] and the pseudopotential approach,[4] the crystal energy can be written in a momentum-space representation:[5]

$$E/\text{atom} = Z\bar{\varepsilon} + E_{xc}(\mathbf{G}=0) + \gamma_{\text{Ewald}} + Z\alpha$$
$$- \tfrac{1}{2}\Omega \sum_{\mathbf{G}(\neq 0)}' V_H(\mathbf{G})\rho(\mathbf{G})$$
$$+ \Omega \sum_{\mathbf{G}(\neq 0)}' [E_{xc}(\mathbf{G}) - V_{xc}(\mathbf{G})]\rho(\mathbf{G}) , \qquad (2)$$

where Z is the number of valence electrons, $\bar{\varepsilon}$ is the mean eigenvalue averaged over all the occupied states; the eigenvalues are calculated with the average potential set to zero.[5] Ω is the atomic volume, $V_H(\mathbf{G})$ is the Hartree potential, $\rho(\mathbf{G})$ is the charge density, and γ_{Ewald} is the Ewald energy. The pseudopotential term α is defined to be

$$\alpha = \frac{1}{\Omega}\int \left[V_{\text{ion}}(r) + \frac{Ze^2}{r} \right] d^3r \equiv \frac{V_{\text{ps}}(\mathbf{G}=0)}{\Omega} , \qquad (3)$$

where $V_{\text{ion}}(r)$ is the ionic pseudopotential. The α term represents only the integrated effect of the pseudopotential. Higher-order effects of the pseudopotential are implicitly contained in $\bar{\varepsilon}$ and $\rho(\mathbf{G})$. For systems where the band structure is not too far from the free-electron dispersion, it is useful to write $\bar{\varepsilon} = \bar{\varepsilon}_0 + \bar{\varepsilon}'$, where $\bar{\varepsilon}_0$ is the average eigenvalue from the free-electron dispersion and $\bar{\varepsilon}'$ is the correction term. The unprime quantities in Eq. (2), $Z\bar{\varepsilon}_0 + E_{xc}(\mathbf{G}=0) + \gamma_{\text{Ewald}} + Z\alpha$, correspond to the energy of a uniform electron density interacting with a periodic array of pseudoions. The prime quantities, including $\bar{\varepsilon}'$, are called the band-structure term, E_{BS}.[6] For semiconductors, $\bar{\varepsilon}'$ contains both effects which can be described by perturbation theory and the fundamental gap which cannot be described by perturbation.

The uniform density term has the following explicit dependence on the Wigner-Seitz radius R:[7]

$$E/\text{atom} = \frac{B}{R^2} - \frac{A}{R} + \frac{C}{R^3} , \qquad (4)$$

where the first term is $Z\bar{\varepsilon}_0$ and $B=\frac{3}{5}(9\pi/4)^{2/3}Z^{5/3}\simeq2.21Z^{5/3}$. The second term includes both the exchange and the Ewald energies and

$$A=(3/2\pi)(9\pi/4)^{1/3}Z^{4/3}+F_s\simeq0.916Z^{4/3}+F_s \ ,$$

where F_s is the structure-dependent Ewald constant. For the diamond structure $F_s=1.671Z^2$. The correlation energy has a very weak dependence on R and hence it is neglected. The third term is $Z\alpha$ and $C=(3/4\pi)V_{\mathrm{ps}}(\mathbf{G}=0)Z$. The numerical values for A, B, and C are in rydberg atomic units. The uniform density term was used previously to examine the bulk moduli of sp metals.[7] It was found that this term alone is adequate to describe metals with small valency but the agreement worsens with increasing valency. The reason is that the charge density is far from uniform for high-valency materials. The uniform density term overestimates the bulk modulus for high-valency materials. One can view the effect of increasing valency both in real space and momentum space. As the valency increases, the pseudopotential becomes more attractive and pulls the charge more toward the core region, hence reducing the number of electrons available for bonding. The modulus generally increases with the valency but not as fast as predicted by the uniform density term. This situation manifests itself in a less transparent but equivalent way in momentum space. As the valency increases, the band-structure term becomes important. It will be shown that the band-structure term has a negative curvature as a function of R, hence it reduces the bulk modulus from the uniform density value.

The band-structure term will be investigated using perturbation theory following Heine and Weaire.[6] The contribution from the fundamental gap is discussed later. Up to second order in perturbation theory, the band-structure term is given by[6]

$$E_{\mathrm{BS}}=\sum_{\mathbf{G}(\neq0)}{}' \ |V(\mathbf{G})|^2|S(\mathbf{G})|^2\mathcal{X}(\mathbf{G})\epsilon(\mathbf{G}) \ , \tag{5}$$

where $V(\mathbf{G})$ is the screened pseudopotential form factor, $S(\mathbf{G})$ is the structure factor, and $\mathcal{X}(\mathbf{G})$ is the susceptibility which is defined as

$$\mathcal{X}(\mathbf{G})=\frac{1}{N}\sum_{\mathrm{spin}}\sum_{k\leq k_f}\frac{1}{k^2-(\mathbf{k}+\mathbf{G})^2} \ , \tag{6}$$

where N is the number of atoms in the crystal. The analytic expression for $\mathcal{X}(\mathbf{G})$ is

$$\mathcal{X}(\mathbf{G})=-\tfrac{1}{2}Z(\tfrac{2}{3}E_f)^{-1}F\left[\frac{G}{2k_f}\right] \ , \tag{7}$$

where

$$F(x)=\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right| \ . \tag{8}$$

The dielectric function $\epsilon(\mathbf{G})$ is related to $\mathcal{X}(\mathbf{G})$,

$$\epsilon(\mathbf{G})=1-\frac{4\pi e^2}{G^2}\left[\frac{2}{\Omega}\right]\mathcal{X}(\mathbf{G})[1-f_{\mathrm{xc}}(\mathbf{G})] \ , \tag{9}$$

where $f_{\mathrm{xc}}(\mathbf{G})$ is a factor which includes the exchange-

correlation effect. We must examine the R dependence of $V(\mathbf{G})$, $\mathcal{X}(\mathbf{G})$, and $\epsilon(\mathbf{G})$ in order to determine the R dependence of the band-structure term. Since $\mathcal{X}(\mathbf{G})$ approaches zero rapidly for large $\mathbf{G}$, it is convenient to consider a one-$\mathbf{G}$ model. For example, the first $\mathbf{G}$ in the diamond or zinc-blende structure is $\mathbf{G}=(1,1,1)2\pi/a$. The potential form factor is defined as

$$V(\mathbf{G})=\frac{1}{\Omega}v(\mathbf{G}) \tag{10}$$

where $v(\mathbf{q})$ is the Fourier transform of the potential. The potential form factor depends on R through both the explicit volume dependence and through its argument. A typical $v(\mathbf{q})$ is shown in Fig. 1. For the $\mathbf{G}=(1,1,1)2\pi/a$, the two dependence nearly cancel each other; if the volume is decreased the Ω^{-1} factor increases but $v(\mathbf{q})$ decreases. Hence, $V(\mathbf{G})$ is nearly R independent for the $\mathbf{G}=(1,1,1)2\pi/a$. The susceptibility $\mathcal{X}(\mathbf{G})$ is proportional to R^2 which is evident from its definition. The dielectric function is proportional to $1+\beta R$ where β is usually a very small number, hence $\epsilon(\mathbf{G})$ is nearly R independent. In conclusion, the R dependence of the band-structure term comes mainly from $\mathcal{X}(\mathbf{G})$ and it is proportional to R^2. The total energy therefore has the following analytic form:

$$E/\mathrm{atom}=\frac{B}{R^2}-\frac{A}{R}+\frac{C}{R^3}-DR^2 \ , \tag{11}$$

where $D\propto|V(\mathbf{G})|^2$ is a positive number. It should be pointed out that the R dependence of the band-structure term is valid only for small deviations from the equilibrium volume; otherwise, the energy approaches negative infinity at large R. Furthermore, a weak pseudopotential is assumed such that second-order perturbation theory is adequate. The validity of the second-order perturbation theory for the structural energy was addressed by Heine and Weaire.[6] They examined the band-structure term when both the lower and upper states were filled. Since both the lower and upper states are summed, the divergences from the second-order perturbation theory cancel. The perturbative result differs from the exact result in the fourth order of the pseudopotential.[6]

We examined the contribution to the band-structure term from the fundamental gap where only the lower state is occupied. The energy of the highest occupied valence band is lowered by $V(2,2,0)$ through degenerate perturbation in addition to contributions given by second-order
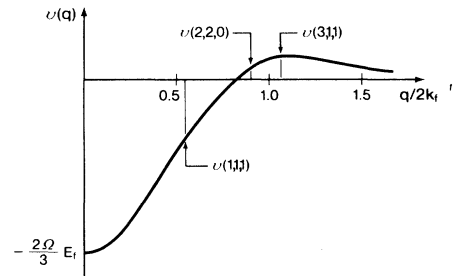

FIG. 1. Typical Fourier transform of screened pseudopotential. The first few $\mathbf{G}$ vectors for the zinc-blende structure are indicated.

perturbation. However, $V(2,2,0)$ is usually nearly zero for most materials in the diamond and zinc-blende structure;[8] therefore, the major effect of the pseudopotential is contained in the perturbation term even for semiconductors.

Using Eq. (11) for the total energy, the bulk modulus can readily be calculated

$$B_0 = \frac{1}{9\Omega_0}\left[\frac{2A}{R_0} - \frac{2B}{R_0^2} - 10DR_0^2\right],\tag{12a}$$

or

$$B_0 = \frac{1}{9\Omega_0}\left[\frac{8B}{R_0^2} - \frac{3A}{R_0} + \frac{15C}{R_0^3}\right],\tag{12b}$$

where R_0 and Ω_0 are the equilibrium Wigner-Seitz radius and equilibrium atomic volume. The equilibrium condition is used either to eliminate the dependence on C [Eq. (12a)] or the dependence on D [Eq. (12b)]. Equation (12) is in Ry/(a.u.)^3. The conversion to GPa is Ry/(a.u.)$^3 = 14\,700$ GPa. Equation (12a) reduces to the uniform density result[7] when $D = 0$. The pressure derivative of B_0 is given by

$$\begin{aligned}B_0' \equiv \left[\frac{dB}{dp}\right]_{p=0} &= 1 - \frac{R_0 E'''}{3E'''} \\ &= \frac{10}{3} + \frac{\dfrac{10}{9\Omega_0}DR_0^2 - \dfrac{2}{27\Omega_0}\dfrac{B}{R_0^2}}{B_0}.\end{aligned}\tag{13}$$

For most materials,

$$\frac{2}{27\Omega_0}\frac{B}{R_0^2} \ll \frac{10}{9\Omega_0}DR_0^2.$$

III. ELEMENTS

The constants A and B are universal functions of the valence charge. The two material parameters of this model are C and D, which are derivable from the pseudopotential. The band-structure term D can be calculated from empirical pseudopotential form factors. For example, the empirical pseudopotential form factor for Si is $V(1,1,1) = -0.21$ Ry,[8] R_0 is 3.18 a.u., and $D = 0.077$ Ry/(a.u.)^2 calculated within the one-G model [using Eqs. (5), (7), (8), and (9) with $f_{xc} = 0.5$].[6] Using Eq. (12a) and (13), we obtain $B_0 = 100$ GPa and $B_0' = 4.3$ for Si while the experimental values[9] are 98 GPa and 4.24, respectively. In principle, given a pseudopotential, we can obtain D or C and hence calculate B_0 and B_0'. This is not the program that we will follow here because we are interested in trends and simple relationships between B_0 and R_0.

In order to compare Eq. (12) with the empirical relation, Eq. (1), for the bulk modulus, we must examine how the average pseudopotential term C or the band-structure term D varies with materials. Empirically, for a given valency, B_0 depends only on R_0. This implies that C and D can be expressed as functions of R_0. This turns out to be so and it can be illustrated using the Ashcroft empty core pseudopotential.[10] For the Ashcroft potential,

$V_{ps}(G=0) = 4\pi Z^2 r_c^2$ or $C = 3Z^2 r_c^2$. The Wigner-Seitz radius varies linearly with r_c, $r_c = a(R_0 - b)$.[7] The coefficients a and b depend on the valency, $a \simeq 0.5$ and $b \simeq 1$ in atomic units. The coefficient b is needed because R_0 is finite even when r_c is zero. For the group-IV materials, we adjusted a and b to fit the bulk moduli and obtained $a = 0.48$ and $b = 1.14$. Therefore, for $Z = 4$, $A \simeq 32.6$, $B \simeq 22.3$, $C = 48r_c^2 \simeq 11(R_0 - 1.14)^2$. Substituting these values in Eq. (12b) gives

$$B_{0,\text{IV}} = \frac{1}{9\Omega_0}\left[\frac{178}{R_0^2} - \frac{98}{R_0} + \frac{166(R_0 - 1.14)^2}{R_0^3}\right]47000 \text{ GPa}.\tag{14}$$

Although Eq. (14) does not resemble the simple power law of the empirical formula, Eq. (1) with $\lambda = 0$, it does give similar numerical values for the bulk moduli, see Table I. Equation (14) expresses the bulk modulus as a sum of competing terms, the kinetic energy, the exchange and Ewald energies, and the pseudopotential core-size term. The magnitudes of these terms are comparable. Although each term has an exponent greater than 3.5, the terms nearly cancel each other to give a weaker exponent.

The pressure derivative of the bulk modulus can be calculated from Eq. (13). The value for D can be obtained from C through the equilibrium condition or from the bulk modulus by inverting Eq. (12a). For the group-IV materials, the band-structure correction to the bulk modulus, $10/9\Omega_0 DR_0^2$, is of order of the bulk modulus, therefore B_0' is between 4 and 5, see Table I. One further point worth noting is that the predicted bulk modulus for Ge is quite a bit different from the experimental value in comparison with the other group-IV materials. We are not certain of the exact cause for this discrepancy at present, but it is possible that the d states are affecting the bulk modulus. On the other hand, the bulk modulus of GaAs is well described by the present approach without invoking the d states, see Sec. IV A and Table I.

IV. COMPOUNDS

It was argued[1] that the effect of ionicity is to reduce the amount of bonding charge and hence reduce the bulk modulus. This picture is essentially consistent with the present results. The reduction of the bond charge is related to the band-structure term. In an AB compounds, this term gets larger because it is proportional to both the symmetric and antisymmetric form factors $|V_s(G)|^2 + |V_a(G)|^2$. To analyze the ionicity effect, it is useful to write

$$\begin{aligned}A &= A_{\text{IV}} + A', \\ C &= C_{\text{IV}} + C', \\ D &= D_{\text{IV}} + D',\end{aligned}\tag{15}$$

where A_{IV}, C_{IV}, and D_{IV} are the parameters for the covalent group-IV material and the prime quantities are ionic parameters. The valency Z is the average valency of atoms A and B. The difference between D and D' is the asymmetric potential. The parameter

$$C = (3/4\pi)Z^{\frac{1}{2}}[V_{ps}^A(\mathbf{G}=0) + V_{ps}^B(\mathbf{G}=0)] .$$

The difference between A and A' comes from the Ewald energy. The Ewald energy of an AB compound is equal to the Ewald energy of the group-IV plus a Madelung energy. $A' = 1.1734(\Delta Z)^2$ for zinc-blende structure where $\Delta Z = (Z_A - Z_B)/2 = 1$ and 2 for III-V and II-VI semiconductors, respectively. The total energy is then separated into the covalent energy, E_{IV}, and the ionic contributions

$$E = E_{IV} - \frac{A'}{R} + \frac{C'}{R^3} - D'R^2 . \tag{16}$$

The bulk modulus is given by

$$B_0 = B_{0,IV} - \frac{1}{9\Omega}\left[\frac{2A'}{R_0} + 2D'R_0^2 - \frac{12C'}{R_0^3}\right] . \tag{17}$$

A. III-V compounds

We will show that the bulk modulus of a III-V compound can be calculated given the bulk modulus of the group IV compounds. We use an empirical fact that the lattice constant of a III-V compound is the same as its group-IV counterpart. This means that if we differentiate Eq. (16) and set it equal to zero, the derivative of the co-

valent and ionic terms are zero separately. For III-V compounds $C' \cong 0$, therefore D' is related to A' by

$$D' = \frac{A'}{2R_0^3} . \tag{18}$$

Substituting this value for D' in the bulk modulus equation, Eq. (17), gives

$$B_0 = B_{0,IV} - \frac{1}{3}\frac{A'}{\Omega_0 R_0} . \tag{19}$$

Since A' is known, Eq. (19) enables one to calculate the bulk modulus for a III-V compound given $B_{0,IV}$. For skew compounds, we can use the empirical formula given by Eq. (1) with $\lambda = 0$ or Eq. (14) for $B_{0,IV}$. For simplicity we will use Eq. (1). Equation (19) is rewritten as

$$B_0 = \frac{1971}{d^{3.5}} - \frac{408(\Delta Z)^2}{d^4} , \tag{20}$$

where B_0 is in GPa and d is in Å. This formula is appropriate for zinc-blende structure. We should emphasize that the numerical factor 408 is not an empirical coefficient, it comes from the Madelung constant A'. The agreement between Eq. (20) and the experimental values is

TABLE I. Comparison of calculated and measured values of bulk moduli B_0 and its pressure derivative B_0'. The bulk moduli are calculated (a) using Eq. (14) for the group-IV compounds and Eq. (20) with ΔZ equal to 1 and 2 for III-V and II-VI compounds, respectively, (b) using empirical relation Eq. (1), and (c) using Eq. (22) with $V_{ps}(\mathbf{G}=0) \propto 1/Z^{0.5}$. The pressure derivative B_0' is calculated with Eq. (13) using the experimental value for B_0.

	d (Å)	B(expt) (GPa)	B(calc) (a)	B(calc) (b)	B(calc) (c)	B_0' (expt)	B_0' (calc)
			Group IV				
C	1.55	442	436.9	430.1		4.69	4.4
SiC	1.88	211	208.6	215.7			4.4
Si	2.35	98	100.0	99.1		4.24	4.3
Ge	2.45	77.2	87.6	85.8		4.55	4.5
α-Sn	2.81	53	55.9	52.7			4.2
			Group III-V				
BN	1.57	367.0	342.3	364.3	358.0		4.8
BP	1.97	165.0	158.0	164.6	167.9		4.7
AlP	2.36	86.0	84.0	86.2	89.9		4.6
AlAs	2.43	77.0	76.1	77.9	81.5		4.6
AlSb	2.66	58.2	56.4	57.3	60.5	4.55	4.5
GaP	2.36	88.7	84.5	86.7	90.4	4.77	4.6
GaAs	2.45	74.8	74.5	76.3	79.8	4.67	4.6
GaSb	2.65	57.0	56.9	57.9	61.0	4.8	4.5
InP	2.54	71.0	65.6	67.0	70.3	4.9	4.5
InAs	2.61	60.0	59.5	60.6	63.9	4.8	4.5
InSb	2.81	47.4	46.7	47.4	50.2	4.9	4.5
			Group II-IV				
ZnS	2.34	77.1	44.7	77.9	70.4	4.7	5.4
ZnSe	2.45	62.4	39.1	66.0	61.2	5.1	5.5
ZnTe	2.64	51.0	32.3	51.4	49.4		5.3
CdS	2.52	62.0	36.5	60.3	56.7		5.3
CdSe	2.62	53.0	32.8	52.6	50.4		5.3
CdTe	2.81	42.4	27.5	41.4	40.8		5.1
HgSe	2.63	50.0	32.4	51.6	49.5		5.3
HgTe	2.78	42.3	28.1	42.5	41.8		5.2

very good for the III-V compounds except those with elements from the upper rows of the Periodic Table; see Table I, column (a).

B. II-VI compounds

For II-VI compounds, using Eq. (20) with $\Delta Z = 2$ would not give the correct bulk modulus; see Table I, column (a). The reason for this is that in deriving Eq. (20) it was assumed that $C \cong C_{IV}$ or $C' \cong 0$. This is not true for II-VI compounds. Recall that

$$C = (3/4\pi)Z^{\frac{1}{2}}[V_{ps}^A(\mathbf{G}=0) + V_{ps}^B(\mathbf{G}=0)] .$$

An atom with a high valency has a small $V_{ps}(\mathbf{G}=0)$; that is, a high valency atom is more electronegative. For the Ashcroft pseudopotential, $V_{ps}(\mathbf{G}=0) = 4\pi Z r_c^2$. The core radius r_c decreases with increasing Z. One would expect $V_{ps}(\mathbf{G}=0)$ to scale as $V_{ps}(\mathbf{G}=0) \propto Z^p$, where p is a negative number. This scaling ignores variations between rows in the Periodic Table. Expanding $V_{ps}(\mathbf{G}=0)$ about $Z = 4$, one obtains

$$C' + \frac{p(p-1)}{2}\left[\frac{\Delta Z}{Z}\right]^2 C_{IV} . \tag{21}$$

The bulk modulus is given by

$$B_0 = B_{0,IV} - \frac{1}{3}\frac{A'}{\Omega_0 R_0} + \frac{5}{3}\frac{C'}{\Omega_0 R_0^3} . \tag{22}$$

The value of C_{IV} can be obtained from $B_{0,IV}$ by inverting Eq. (12b) or from $C_{IV} \simeq 11(R_0 - 1.14)^2$ and C' is calculated from Eq. (21). We find that $p \simeq -0.5$ gives good results for the II-VI compounds; see Table I, column (c), but it worsens some of the agreements for the III-V compounds.

V. CONCLUSIONS

Starting with the pseudopotential total-energy formalism, analytic expressions for the bulk modulus and its pressure derivative are derived using perturbation theory and a one-G model. For a given valency, the bulk modulus can be expressed as a function of the Wigner-Seitz radius, R_0, alone because the pseudopotential core radius also scales with R_0. The formulas derived here give similar numerical values for the bulk moduli as the empirical relation. One major difference is that the effect of ionicity enters as ΔZ^2 in the present approach but linear in ΔZ in the empirical relation, λ in Eq. (1) is same as ΔZ. In the present approach the ionic compounds are treated as a small perturbation from the covalent group IV. The quadrative behavior is expected for small ΔZ but higher-order effects of the pseudopotential would weaken the quadratic effect for large ΔZ. Including higher-order effects of the pseudopotential would also improve the agreement for the compounds with elements from the upper rows of the Periodic Table.

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