

Möbius inversion transform for diamond-type materials and phonon dispersions

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In the present paper the Möbius inversion theorem in number theory is applied to diamond-type materials and a transform formula of the pair potential from the cohesive energy is proposed and proved. Then the phonon dispersions of these materials are calculated by the use of the calculated pair potentials. The results show that a three-body interaction is needed to agree with the experimental data. The present work indicates that the Möbius theorem can be used for diamond-type materials.

I. INTRODUCTION

A few years ago it was hard to believe that the Möbius inversion theorem, an old one in number theory, could be used to solve physical problems. In 1990 this theorem was applied to a few inversion problems in physics by Chen.¹ Since then a series of works have appeared to solve the inversion problems in Bose and Fermi systems, lattices, and astrophysics.²⁻⁶ In particular, based on this theorem, the Möbius transform formulas for sc, fcc, bcc, and two-dimensional (2D) hcp structures have been successfully obtained and the solutions of the inverse problems in these structures, from the cohesive energy to the pair potential between atoms, have been given. The properties of some materials have been studied using the pair potentials obtained.⁷⁻¹¹ In the present work a proper formalism of the Möbius transform for diamond-type materials is proposed. By the use of the formula the pair potential of these materials can be obtained from their cohesive energy. This procedure will give a useful way to study the properties of diamond-type materials, which are important materials. In illustration of the method numerical calculations of the pair potential for diamond, silicon, germanium, and gray tin first are carried out. Then the phonon dispersions of these materials are calculated using the calculated pair potentials. In order to agree with experiments the Slater-Kirkwood three-body interaction is considered in the above calculations. At the end the results are compared with inelastic neutron scattering data. In Sec. II the expression for the cohesive energy is obtained. The Möbius inversion formula for diamond-type materials is given and proved in Sec. III. The numerical calculations of the pair potential for diamond, silicon, germanium, and gray tin are

presented in Sec. IV. In Sec. V the phonon dispersions are evaluated and the results are discussed in Sec. VI.

II. THE COHESIVE ENERGY FOR DIAMOND-TYPE MATERIALS

It is well known that the cohesive energy per atom of a crystal can be expressed as

$$E(r) = \frac{1}{2} \sum_i \phi^{(2)}(\mathbf{r}_i) + \frac{1}{3!} \sum_{i,j} \phi^{(3)}(\mathbf{r}_i, \mathbf{r}_j) + \dots, \quad (1)$$

where r is the lattice constant and \mathbf{r}_i and \mathbf{r}_j are the position vectors of the i th and j th atoms from the one at the origin, respectively. $\phi^{(2)}$ and $\phi^{(3)}$ represent the two-body and three-body interactions. In the first approximation we just consider the two-body interaction for the cohesive energy $E(r)$,

$$E(r) = \frac{1}{2} \sum_i \phi^{(2)}(\mathbf{r}_i) = \frac{1}{2} \sum_{|\mathbf{r}_i| \neq 0} \phi^{(2)}(|\mathbf{r}_i|). \quad (2)$$

For diamond-type materials the lattice consists of two interpenetrating face-centered cubic Bravais lattices, displaced along the body diagonal of the cubic cell by one-quarter the length of the diagonal. Therefore the cohesive energy can be considered as a sum of two parts. One of them contains the contribution of the fcc lattice atoms and the other the contribution of the atoms located at the body diagonals:

$$E(r) = E_{\text{fcc}}(r) + E_{\text{dia}}(r). \quad (3)$$

The former is⁴

$$E_{\text{fcc}}(r) = 3 \sum_{n=1}^{\infty} \phi(nr) + 6 \sum_{p,q=1}^{\infty} [\phi(\sqrt{p^2+q^2}r) + \phi(\sqrt{(p-\frac{1}{2})^2+(q-\frac{1}{2})^2}r)] \\ + 4 \sum_{p,q,u=1}^{\infty} [\phi(\sqrt{p^2+q^2+u^2}r) + 3\phi(\sqrt{(p-\frac{1}{2})^2+(q-\frac{1}{2})^2+u^2}r)] \quad (4)$$

and the latter

$$E_{\text{dia}}(r) = 2 \sum_{p,q,t=1}^{\infty} \left\{ \phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{1}{4})^2+(t-\frac{1}{4})^2}r) + 3\phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{1}{4})^2+(t-\frac{3}{4})^2}r) \right. \\ \left. + 3\phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{3}{4})^2+(t-\frac{3}{4})^2}r) + \phi(\sqrt{(p-\frac{3}{4})^2+(q-\frac{3}{4})^2+(t-\frac{3}{4})^2}r) \right\}. \quad (5)$$

In Eq. (4) the first sum represents the contribution of the atoms located on the three axes to the cohesive energy. The second sum is the contribution of the atoms in axial planes. The third one comes from other atoms. In Eq. (5) E_{dia} denotes the contribution from four kinds of atoms located on the diagonals.

III. THE MÖBIUS INVERSE-TRANSFORM FORMULA FOR DIAMOND-TYPE MATERIALS

We can divide the cohesive energy $E(r)$ into two parts, $E_0(r)$ and $E_1(r)$,

$$E(r) = E_0(r) + E_1(r), \quad (6)$$

where

$$E_0(r) = \sum_{n=1}^{\infty} \left\{ 3\phi(nr) + 6\phi(\sqrt{2}nr) + 6\phi\left[\frac{(2n-1)}{\sqrt{2}}r\right] + 4\phi(\sqrt{3}nr) + 2\phi[(n-\frac{1}{4})\sqrt{3}r] + 2\phi[(n-\frac{3}{4})\sqrt{3}r] \right\} \\ = \sum_{n=1}^{\infty} \left\{ 3\phi(nr) + 6\phi\left[\frac{2n}{\sqrt{2}}r\right] + 6\phi\left[\frac{2n-1}{\sqrt{2}}r\right] + 2\phi(\sqrt{3}nr) + 2\phi[(n-\frac{1}{4})\sqrt{3}r] + 2\phi[(n-\frac{3}{4})\sqrt{3}r] \right. \\ \left. + 2\phi[(n-\frac{3}{4})\sqrt{3}r] + \phi\left[\frac{\sqrt{6}}{4}nr\right] + \left[2\phi(\sqrt{3}nr) - 2\phi[(n-\frac{3}{4})\sqrt{3}r] - \phi\left[\frac{\sqrt{6}}{4}nr\right] \right] \right\} \quad (7)$$

and

$$E_1(r) = 6 \sum_{p \neq q=1}^{\infty} [\phi(\sqrt{p^2+q^2}r) + \phi(\sqrt{(p-\frac{1}{2})^2+(q-\frac{1}{2})^2}r)] \\ + 2 \sum_{p \neq q \neq t=1}^{\infty} [2\phi(\sqrt{p^2+q^2+t^2}r) + \phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{1}{4})^2+(t-\frac{1}{4})^2}r) + \phi(\sqrt{(p-\frac{3}{4})^2+(q-\frac{3}{4})^2+(t-\frac{3}{4})^2}r)] \\ + 6 \sum_{p,q,t=1}^{\infty} \{ 2\phi(\sqrt{(p-\frac{1}{2})^2+(q-\frac{1}{2})^2+t^2}r) + \phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{1}{4})^2+(t-\frac{3}{4})^2}r) \\ + \phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{3}{4})^2+(t-\frac{3}{4})^2}r) \}. \quad (8)$$

From Eq. (7) it is clear that $E_0(r)$ contains all of the diagonal terms of the first two sums and the diagonal terms of the first part of the third sum in Eq. (4). In addition, it also contains those of the first and fourth sums in Eq. (5). $E_1(r)$ represents the other terms in Eqs. (4) and (5).

We introduce operators R_0 and J which are defined as

$$R_0\phi(r) = \sum_{n=1}^{\infty} \left\{ 3\phi(nr) + 6\phi\left[\frac{2n}{\sqrt{2}}r\right] + 6\phi\left[\frac{2n-1}{\sqrt{2}}r\right] + 2\phi(\sqrt{3}nr) + 2\phi[(n-\frac{1}{4})\sqrt{3}r] \right. \\ \left. + 2\phi[(n-\frac{3}{4})\sqrt{3}r] + 2\phi[(n-\frac{3}{4})\sqrt{3}r] + \phi\left[\frac{\sqrt{6}}{4}nr\right] \right\} \\ = \sum_{n=1}^{\infty} \left\{ 3\phi(nr) + 6\phi\left[\frac{1}{\sqrt{2}}nr\right] + 2\phi\left[\frac{4n}{4}\sqrt{3}r\right] \right. \\ \left. + 2\phi\left[\frac{4n-1}{4}\sqrt{3}r\right] + 2\phi\left[\frac{4n-2}{4}\sqrt{3}r\right] + 2\phi\left[\frac{4n-3}{4}\sqrt{3}r\right] + \phi\left[\frac{\sqrt{6}}{4}nr\right] \right\} \\ = \sum_{n=1}^{\infty} \left\{ 3\phi(nr) + 6\phi\left[\frac{1}{\sqrt{2}}nr\right] + 2\phi\left[\frac{\sqrt{3}}{4}nr\right] + \phi\left[\frac{\sqrt{6}}{4}nr\right] \right\}, \quad (9)$$

$$\begin{aligned}
J\phi(r) = & 6 \sum_{p \neq q=1}^{\infty} [\phi(\sqrt{p^2+q^2}r) + \phi(\sqrt{(p-\frac{1}{2})^2+(q-\frac{1}{2})^2}r)] \\
& + 2 \sum_{p \neq q \neq t=1}^{\infty} [2\phi(\sqrt{p^2+q^2+t^2}r) + \phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{1}{4})^2+(t-\frac{1}{4})^2}r) \\
& \quad + \phi(\sqrt{(p-\frac{3}{4})^2+(q-\frac{3}{4})^2+(t-\frac{3}{4})^2}r)] \\
& + 6 \sum_{p,q,t=1}^{\infty} [2\phi(\sqrt{(p-\frac{1}{2})^2+(q-\frac{1}{2})^2+t^2}r) + \phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{1}{4})^2+(t-\frac{3}{4})^2}r) \\
& \quad + \phi(\sqrt{(p-\frac{1}{4})^2+(q-\frac{3}{4})^2+(t-\frac{3}{4})^2}r)] \\
& + 2 \sum_{n=1}^{\infty} \left\{ \phi(\sqrt{3}nr) - \phi[(n-\frac{1}{2})\sqrt{3}r] - \frac{1}{2}\phi\left[\frac{\sqrt{6}}{4}nr\right] \right\}. \tag{10}
\end{aligned}$$

The cohesive energy can be expressed in terms of R_0 , J , and $\phi(r)$ as

$$E(r) = (R_0 + J)\phi(r) = R_0(1 + R_0^{-1}J)\phi(r). \tag{11}$$

Making an inverse operation we have

$$\phi(r) = (1 + R_0^{-1}J)^{-1}R_0^{-1}E(r). \tag{12}$$

Therefore the pair potential $\phi(r)$ can be obtained from the cohesive energy $E(r)$ directly. So the problem of solving the pair potential from the cohesive energy becomes how to get the operator R_0^{-1} .

In number theory,¹² there is a Möbius theorem which states that for $x > 0$, if

$$F(x) = \sum_{n=1}^{\infty} f(nx), \tag{13}$$

then

$$f(x) = \sum_{n=1}^{\infty} \mu(n)F(nx) \tag{14}$$

and vice versa, provided

$$\sum_{m,n} |f(mnx)| \tag{15}$$

converges. Here $F(x)$ and $f(x)$ are real functions and $\mu(n)$ is known as the Möbius function defined as follows:

$$\mu(n) = \begin{cases} 1 & \text{for } n = 1, \\ 0 & \text{if } n \text{ includes repeat factors,} \\ (-1)^k & \text{if } n \text{ is a product of } k \text{ distinct primes.} \end{cases} \tag{16}$$

By the use of the Möbius theorem and Eq. (9) it can be proved that for a real function $f(r)$

$$R_0^{-1}f(r) = -\frac{1}{6} \sum_{m,n,u=1}^{\infty} (-3)^m (-\frac{1}{2})^u {}^{-1}\mu(n) f\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}nr\right], \tag{17}$$

where $\mu(n)$ is the Möbius function. The proof is as follows.

$$\begin{aligned}
R_0^{-1}R_0\phi(r) &= R_0^{-1} \sum_{s=1}^{\infty} \left\{ 3\phi(sr) + 6\phi\left[\frac{1}{\sqrt{2}}sr\right] + 2\phi\left[\frac{\sqrt{3}}{4}sr\right] + \phi\left[\frac{\sqrt{6}}{4}sr\right] \right\} \\
&= \sum_{s=1}^{\infty} \sum_{m,n,u=1}^{\infty} -\frac{1}{6}(-3)^m(-\frac{1}{2})^{u-1}\mu(n) \\
&\quad \times \left\{ 3\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}nsr\right] + 6\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}n\frac{1}{\sqrt{2}}sr\right] + 2\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}n\frac{\sqrt{3}}{4}sr\right] \right. \\
&\quad \left. + \phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}n\frac{\sqrt{6}}{4}sr\right] \right\} \\
&= \sum_{m,n,u,s=1}^{\infty} (-3)^m(-\frac{1}{2})^u\mu(n) \left\{ \phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}nsr\right] + 2\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{(u-1)/2}nsr\right] \right. \\
&\quad \left. + \frac{1}{3}\left\{ \phi\left[\left[\frac{4}{\sqrt{6}}\right]^{m-1} 2^{u/2}nsr\right] + 2\phi\left[\left[\frac{4}{\sqrt{6}}\right]^{m-1} 2^{(u-1)/2}nsr\right] \right\} \right\} \\
&= \sum_{m,n,s=1}^{\infty} \left\{ \sum_{u=1}^{\infty} (-3)^m(-\frac{1}{2})^u\mu(n)\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}nsr\right] \right. \\
&\quad + 2\sum_{u=0}^{\infty} (-3)^m(-\frac{1}{2})^{u+1}\mu(n)\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m 2^{u/2}nsr\right] \left. \right\} \\
&\quad + \frac{1}{3}\left\{ \sum_{u=1}^{\infty} (-3)^m(-\frac{1}{2})^u\mu(n)\phi\left[\left[\frac{4}{\sqrt{6}}\right]^{m-1} 2^{u/2}nsr\right] \right. \\
&\quad \left. + 2\sum_{u=0}^{\infty} (-3)^m(-\frac{1}{2})^{u+1}\mu(n)\phi\left[\left[\frac{4}{\sqrt{6}}\right]^{m-1} 2^{u/2}nsr\right] \right\} \\
&= \sum_{m,n,s=1}^{\infty} \left\{ -(-3)^m\mu(n)\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m nsr\right] - \frac{1}{3}(-3)^m\mu(n)\phi\left[\left[\frac{4}{\sqrt{6}}\right]^{m-1} nsr\right] \right\}, \\
&= \sum_{n,s=1}^{\infty} \mu(n) \left\{ \sum_{m=1}^{\infty} -(-3)^m\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m nsr\right] + \sum_{m=0}^{\infty} (-3)^m\phi\left[\left[\frac{4}{\sqrt{6}}\right]^m nsr\right] \right\} \\
&= \sum_{n,s=1}^{\infty} \mu(n)\phi(ns r). \tag{18}
\end{aligned}$$

From Eqs. (13) and (14) it can be deduced that

$$\begin{aligned}
f(x) &= \sum_{n=1}^{\infty} \mu(n)F(nx) \\
&= \sum_{n=1}^{\infty} \mu(n) \sum_{s=1}^{\infty} f(snx) \\
&= \sum_{n,s=1}^{\infty} \mu(n)f(snx). \tag{19}
\end{aligned}$$

Therefore Eq. (18) becomes

$$R_0^{-1}R_0\phi(r) = \phi(r) \tag{20}$$

and the proof is completed.

By use of Eqs. (10), (12), (16), and (17) the pair potential can be obtained from the cohesive energy $E(r)$:

$$\phi(r) = (1 - R_0^{-1}J + R_0^{-1}JR_0^{-1}J - \dots)R_0^{-1}E(r). \tag{21}$$

Equation (17) is the Möbius transform formula for

diamond-type materials. Combining Eqs. (10), (17), and (21) the inverse problem for diamond-type materials, of going from cohesive energy to pair potential, is solved. This procedure will give a precise method to obtain the pair potential. If the cohesive energy comes from an *ab initio* calculation, this will be a first-principles potential. In the next sections we will give some numerical calculations.

IV. THE NUMERICAL CALCULATIONS OF THE PAIR POTENTIAL FOR DIAMONDS, Si, Ge, AND α -Sn

Based on Eq. (21) the pair potentials for diamond, Si, Ge, and gray tin are evaluated. In this work an empirical expression for the cohesive energy is accepted and assumed to have the Morse potential type,

$$E(r) = U[e^{-2p(r-a_0)} - 2e^{-p(r-a_0)}], \tag{22}$$

where U is the cohesive energy of the equilibrium lattice,

TABLE I. U , a_0 , B , and p of diamond, Si, Ge, and α -Sn.

Material	a_0 (Å)	U (eV)	B (10^{12} dyn/cm 2)	p (10^8 /cm)
Diamond	3.567	7.37	5.450	0.963
Ge	5.658	3.85	0.772	0.632
Si	5.430	4.63	0.988	0.638
α -Sn	6.490	3.14	1.110	0.898

a_0 the equilibrium lattice constant, and p a decay factor. The experimental data have been taken for U and a_0 . The decay factor is deduced from the data of the bulk modulus B . For the diamond structure the relation between p and B is

$$p = \frac{3}{4} \left[\frac{Ba_0}{U} \right]^{1/2} \quad (23)$$

The experimental data for B , a_0 , and U for diamond, silicon, germanium, and gray tin are taken from Ref. 13 and listed with the calculated parameter p in Table I.

In order to save computer time we calculate the inverse coefficients first. So we rewrite Eq. (21) as

$$\phi(r) = \sum_p W_p E(S_p r) \quad (24)$$

and calculate the coefficients W_p and S_p by using Eqs. (10), (12), (16), and (17). The Morse potential decreases rapidly with increasing r . Therefore we just need to consider finite terms in the sum in Eqs. (10), (17), and (21). The calculated results for W_p and S_p are listed in Table II. Using the coefficients W_p and S_p it is very easy to obtain the pair potential from the cohesive energy. The calculated pair potentials for diamond, silicon, germanium, and gray tin are shown in Fig. 1.

V. THE PHONON DISPERSIONS OF DIAMOND-TYPE MATERIALS

The phonon dispersions of diamond-type materials have been studied by many authors.¹⁴⁻²² They have measured the phonon dispersions by inelastic scattering of neutrons and fitted the experimental data by atomic force constants. They have indicated that it is necessary to include up to sixth-neighbor interaction for good fitting. In this work we have calculated the atomic force

TABLE II. The coefficients W_p and S_p .

S_p	W_p	S_p	W_p
2.309 401	0.5000	7.888 106	-3.0000
3.771 236	-1.5000	8.432 740	-3.0000
4.422 166	-1.5000	8.467 805	4.5000
5.333 333	-0.7500	8.709 297	4.5000
5.811 865	-1.5000	8.743 251	-1.5000
6.158 403	4.5000	9.237 604	-1.0000
6.531 972	-1.5000	9.490 737	9.0000
6.928 203	-2.0000	9.521 904	-3.0000
7.221 368	9.0000	9.977 753	-6.0000
7.542 472	-1.5000	10.056 63	-13.500

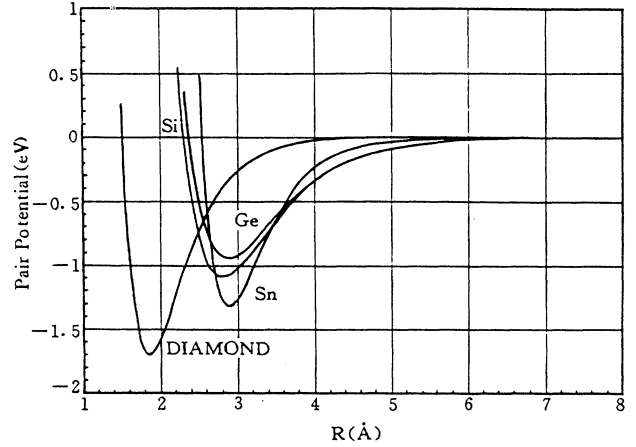


FIG. 1. The pair potentials of diamond, germanium, silicon, and gray tin.

constants up to third neighbor from the calculated pair potentials, and then the phonon dispersions.

According to the Born-von Karman model the total potential Φ of a system can be expressed by the displacement of the atoms away from their equilibrium positions^{23,24} as

$$\begin{aligned} \Phi = & \Phi_0 + \sum_{\alpha, lk} \left[\frac{\partial \Phi}{\partial u_{\alpha, lk}} \right]_0 u_{\alpha, lk} \\ & + \frac{1}{2} \sum_{\alpha, lk \alpha', l' k'} \left[\frac{\partial^2 \Phi}{\partial u_{\alpha, lk} \partial u_{\alpha', l' k'}} \right]_0 u_{\alpha, lk} u_{\alpha', l' k'} \\ & + \dots, \end{aligned} \quad (25)$$

where $u_{\alpha, lk}$ is the α component of the displacement of the k th atom in the l th cell along the α direction.

In the harmonic approximation the vibrational potential of the system is

$$\Phi' = \frac{1}{2} \sum_{\alpha, lk \alpha', l' k'} \left[\frac{\partial^2 \Phi}{\partial u_{\alpha, lk} \partial u_{\alpha', l' k'}} \right]_0 u_{\alpha, lk} u_{\alpha', l' k'}, \quad (26)$$

where $-\left[\partial^2 \Phi / \partial u_{\alpha, lk} \partial u_{\alpha', l' k'} \right]_0$ is known as the atomic force constant. When the pair potential between atoms is known, we can express the potential of the system by the pair potentials

$$\Phi = \frac{1}{2} \sum_i \phi(r_i). \quad (27)$$

Therefore, using the calculated pair potential, the atomic force constants of any neighbors can be obtained immediately. When atoms vibrate around their equilibrium positions the motions of the atoms can be described by the Newton equation

$$M_k \ddot{u}_{alk} = - \sum_{\alpha' l' k'} \left[\frac{\partial^2 \Phi}{\partial u_{alk} \partial u_{\alpha' l' k'}} \right]_0 u_{\alpha' l' k'}, \quad (28)$$

where M_k is the mass of the k th atom and the double overdot represents the second derivative with respect to

time. The solutions of Eq. (28) have the form

$$u_{alk} = \frac{1}{\sqrt{M_k}} A_{\alpha k} e^{i[\mathbf{q} \cdot \mathbf{x}_{lk} - \omega t]}, \quad (29)$$

where $A_{\alpha k}$ is the α component of the amplitude of the vibration of the k th atom, \mathbf{q} the wave vector, \mathbf{x}_{lk} the position vector of the k th atom in the l th cell, and ω the angular frequency of the vibration. Putting Eq. (29) in Eq. (28) we obtain the secular equation

$$\text{Det}[\omega^2 \delta_{\alpha\alpha'} \delta_{kk'} - D_{\alpha\alpha', kk'}(\mathbf{q})] = 0. \quad (30)$$

In Eq. (30) $\delta_{\alpha\alpha'}$ is the Kronecker delta and $D_{\alpha\alpha', kk'}(\mathbf{q})$ is the element of the dynamical matrix

$$D_{\alpha\alpha', kk'}(\mathbf{q}) = \frac{1}{\sqrt{M_k M_{k'}}} \sum_{l'} \left[\frac{\partial^2 \Phi}{\partial u_{alk} \partial u_{\alpha' l' k'}} \right]_0 \times e^{i\mathbf{q} \cdot [\mathbf{x}_{l' k'} - \mathbf{x}_{lk}]} \quad (31)$$

Having solved the secular equation the phonon dispersion is obtained.

As mentioned in our previous work¹⁰ it is not sufficient just to consider the two-body interaction in Eq. (1). Because there are only four nearest neighbors and the outer electron of these materials is a p electron, the anisotropy is remarkable and the three-body interaction must be considered to agree with the experiment in calculating the phonon dispersion. In the present work a Slater-Kirkwood three-body interaction $\phi^{(3)}$ is used,²⁵

$$\phi^{(3)} = [Ae^{-\alpha(r_i + r_j + r_{ij})} + C(r_i r_j r_{ij})^{-3}] \times (1 + 3 \cos \theta_i \cos \theta_j \cos \theta_{ij}), \quad (32)$$

where r_i , r_j , and r_{ij} are three sides of a triangle and θ_i , θ_j , and θ_{ij} are its interior angles. A and C denote the strength of the three-body interaction and α is a decay factor; they are adjustable parameters. In our calculation the three-body interactions up to second-nearest neighbor are taken into account. There are six sets of triangles consisting of two nearest neighbors and a reference atom. Their sides and interior angles are

$$\begin{aligned} r_i = r_j &= \frac{\sqrt{3}}{4} r, \\ r_{ij} &= \frac{1}{\sqrt{2}} r, \\ \theta_i = \theta_j &= 35.2644^\circ, \\ \theta_{ij} &= 109.4712^\circ, \end{aligned} \quad (33)$$

where r is the lattice constant. For second-nearest neighbors there are 24 sets of triangles consisting of two

TABLE III. The adjustable parameters A , C , and α .

Material	A (eV)	C (eV)	α ($10^8/\text{cm}$)
Diamond	-600.3	0.1192	0.6014
Ge	-358.2	0.0006495	0.3567
Si	-272.4	0.0009403	0.3779
α -Sn	-270.5	0.0000948	0.3529

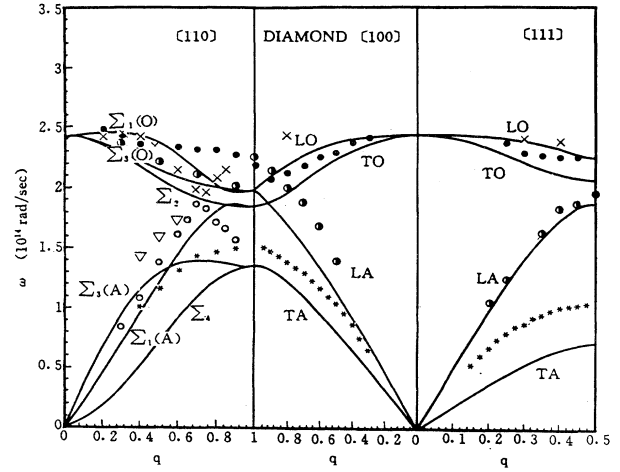


FIG. 2. Comparison of the calculated phonon dispersion with the experimental data for diamond.

second-nearest neighbors and a reference atom. Their sides and interior angles are

$$\begin{aligned} r_i = r_j = r_{ij} &= \frac{1}{\sqrt{2}} r, \\ \theta_i = \theta_j = \theta_{ij} &= 60^\circ. \end{aligned} \quad (34)$$

Considering the three-body interaction Eq. (1) becomes

$$E(r) = \left\{ A \left[\frac{1}{3} e^{-\alpha(\sqrt{2} + \sqrt{3})r/2} + \frac{11}{2} e^{-3\alpha r/\sqrt{2}} \right] + \frac{15320}{81} \sqrt{2} C r^{-9} \right\} = \frac{1}{2} \sum_i \phi^{(2)}(|\mathbf{r}_i|). \quad (35)$$

Using the above developed method a new pair potential can be obtained.

Having properly adjusted the parameters A , C , and α the new atomic force constants are obtained and then the

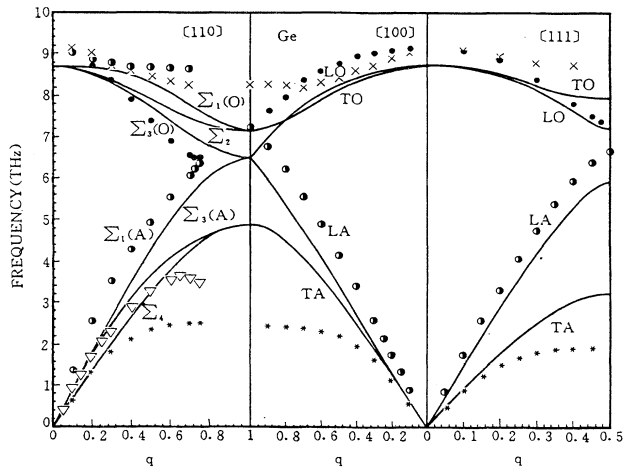


FIG. 3. Comparison of the calculated phonon dispersion with the experimental data for germanium.

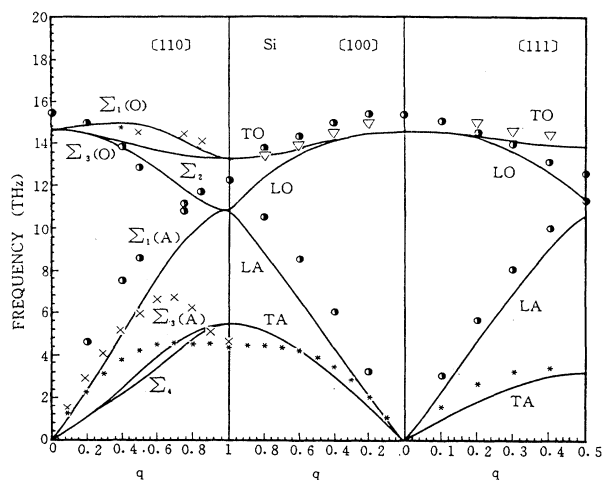


FIG. 4. Comparison of the calculated phonon dispersion with the experimental data for silicon.

elements of the dynamical matrix. Solving secular equation (30) the phonon dispersions in the directions [100], [110], and [111] are calculated. The adjustable parameters are listed in Table III and the calculated phonon dispersions with the experimental data are shown in Figs. 2–5.

VI. DISCUSSIONS AND CONCLUSIONS

The proposed Möbius transform formula in this paper gives a precise method to get the pair potential of diamond-type materials from their cohesive energy. The calculated pair potentials might be useful for studying the properties of the above materials and simulating their behavior. This might be of interest to physicists and materials scientists. In particular, this method can include the effect of many-body interactions, so it can give an effective way to consider their effect on the properties of the above materials.

In Fig. 1 it is shown that the equilibrium distance of a pair potential of a material is smaller than the other's and

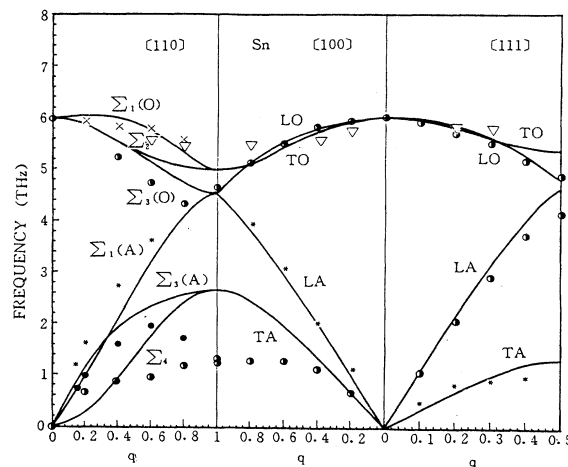


FIG. 5. Comparison of the calculated phonon dispersion with the experimental data for gray tin.

its equilibrium lattice constant is smaller than the other's.

The calculated results of the phonon dispersions for diamond-type materials are in good agreement with the experimental data from inelastic scattering of neutrons. The results also indicate that the three-body interaction is not negligible for calculating the phonon dispersions. But there are some discrepancies between the theory and the experiment, especially in the direction [110] near the zone boundary. There might be two causes for this. First, when we calculate the atomic force constants (AFC's) we only consider the interaction up to the third neighbors, but the AFC's of fifth neighbors are quite important [22]. Secondly, the Morse potential might not be a good expression for the cohesive energy of diamond-type materials.

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