Vol 11 No 4, April 2002
1009-1963/2002/11(04)/0332-07

Chinese Physics

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A general Möbius inversion transform formula for hcp lattices and its application*

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(Received 8 October 2001; revised manuscript received 11 December 2001)

In this paper, we present a general Möbius inversion transform formula for hcp lattices. This formula can be applied to hcp lattices with a non-ideal c/a value and to obtain the pair potential between atoms in these lattices from the cohesive energy. Also, the three-body interaction among atoms in the lattices can be taken into account in the method. This method gives a useful means to obtain interatomic interactions in the interatomic force model. The method has been applied to zinc, and the pair potential obtained is used to calculate the phonon dispersion relations for some high-symmetry directions. It is found that, by properly considering a three-body interaction, one can acquire satisfactory results.

Keywords: lattice theory, interatomic potentials and forces, phonon dispersions
PACC: 0550, 3420, 6320

1. Introduction

It is well known that various first-principle methods have been developed based on quantum mechanics. Using these methods, we can study a variety of properties of condensed matter and understand them at an electron structure level. For complex systems, however, these methods are difficult to use, so the interatomic force model continues to show its value in the physical research of matter. In this model, the key step is to know the interaction among atoms. As the interaction cannot be measured experimentally, some empirical expressions for the interaction have been proposed.[1] In these expressions, there are some parameters which need to be fitted by some physical properties. In 1980, Carlsson *et al.*[2] suggested an inversion method, by which the interaction can be directly calculated from the cohesive energy. In 1992, Chen *et al.*[3] applied the Möbius theorem in the number theory to the lattice inversion problems and greatly improved Carlsson's method. They also gave some inversion transform formulae, by which the pair potentials can be obtained from the cohesive energies for fcc, bcc and two-dimensional (2D) hcp structures. Using Chen's method and the obtained pair potentials, some physical properties of materials with fcc and bcc structures have been studied.[4,5] In this paper, we present a general Möbius inversion transform formula, which can be used for hcp lattices with non-ideal structures, with any value of c/a. A very important fact is that most materials with hcp lattices do not possess the ideal value of c/a, so this method can be extensively applied to all materials with hcp structures. Using this formula, from the cohesive energy we can calculate more exactly the pair potentials between atoms in materials with ideal or non-ideal hcp structures. Moreover, it allows us to consider the effect of the three-body interaction in this method, and this is also important for the hcp-structured materials, in which strong anisotropy exists extensively.

As an illustrative example, we use the above-mentioned formula to compute the interatomic potential in zinc, with which we have studied the property of this material, namely the phonon dispersion relations along the directions of T, T', Δ and Σ. It was found that the results were not satisfactory, because the structure of zinc is strongly non-ideal, whose value of c/a is equal to 1.861, seriously deviating from the ideal value 1.633. Obviously, there is a strong anisotropy in zinc. Therefore, the three-body interaction needs to be considered in the above inversion transform formula. We consider the three-body interaction in the calculation of phonon dispersion relations, as shown in Fig.4, and compare it with experimental data. It is found that the agreement of the

*Project supported by the National Natural Science Foundation of China (Grant No 59771044).

theory with the experiment is acceptable.

2. The cohesive energy of a crystal with hcp structure

In a crystal, there are two-body and many-body interactions among atoms. As a first approximation we consider simply the two-body interaction and neglect the many-body interaction in the cohesion of the crystal. Therefore, the cohesive energy per atom, E, in the crystal can be written as

$$E = \frac{1}{2}\sum_{r}\phi(r), \tag{1}$$

where $\phi(r)$ is the two-body interaction (the pair potential) and r is the distance of an atom away from a reference atom, used as the origin.

The energy E can be expressed as a function of the lattice constant a, i.e. $E = E(a)$.

Therefore, for a hcp lattice, Eq.(1) becomes

$$\begin{aligned} E(a) =& 3\sum_{n=1}^{\infty}\phi(na) + \sum_{n=1}^{\infty}\phi\left(n\sqrt{\frac{p}{3}}a\right) + 3\sum_{m,n=1}^{\infty}\phi(\sqrt{m^2+n^2+mn}a) \\ &+ 6\sum_{m,n,l=1}^{\infty}\phi\left(\sqrt{m^2+n^2+mn+\frac{p}{3}l^2}a\right) + 6\sum_{m,n=1}^{\infty}\phi\left(\sqrt{m^2+\frac{p}{3}n^2}a\right) \\ &+ 3\sum_{m,n,l=1}^{\infty}\phi\left(\sqrt{\left(m-\frac{2}{3}\right)^2+\left(n-\frac{2}{3}\right)^2+\frac{p}{3}\left(l-\frac{1}{2}\right)^2+\left(m-\frac{2}{3}\right)\left(n-\frac{2}{3}\right)}a\right) \\ &+ 3\sum_{m,n,l=1}^{\infty}\phi\left(\sqrt{\left(m-\frac{1}{3}\right)^2+\left(n-\frac{1}{3}\right)^2+\frac{p}{3}\left(l-\frac{1}{2}\right)^2+\left(m-\frac{1}{3}\right)\left(n-\frac{1}{3}\right)}a\right). \end{aligned} \tag{2}$$

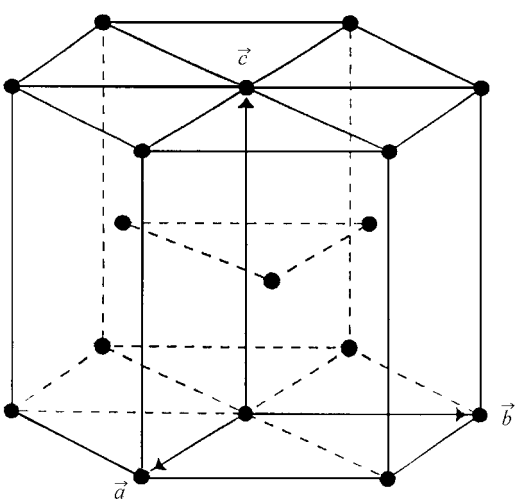


Fig.1. The hcp structure of a crystal. The primitive cell has $\vec{a} = \vec{b}$, with an included angle of 120°. The $\vec{c}$ axis is normal to the plane of $\vec{a}$ and $\vec{b}$, and $\vec{c} = \sqrt{\frac{p}{3}}\vec{a}$. There are two atoms in the cell. One is at the origin and the other at $\vec{r} = \frac{2}{3}\vec{a} + \frac{1}{3}\vec{b} + \frac{1}{2}\vec{c}$.

In Eq.(2), the contribution to the first summation is given by atoms located on the six symmetrical axes in the coordinate plane (see Fig.1), the contribution to the second summation is given by atoms located on the $\vec{c}$ axis. The constant $\vec{c}$ denotes the distance between the origin and the nearest-neighbour atom on this axis. It should be noted that $c/a = \sqrt{\frac{p}{3}}$ is adopted and p is taken as a parameter. Properly choosing the parameter p, we can describe any value of the ratio c/a, i.e. any non-ideal hcp structure. The contribution to the third summation in Eq.(2) is given by atoms in the coordinate plane except those on the symmetrical axes. The fourth summation arises from atoms located outside the coordinate plane and at similar positions as described by the third summation. The fifth summation is contributed by atoms included in the six symmetrical planes except those on the axes. The last two summations are the contributions of the rest atoms.

3. The general Möbius inversion transform formula for hcp lattices

In this section we present the general Möbius inversion transform formula; we give the proof in the Appendix. Firstly, we divide Eq.(2) into two parts

$$E = E_0 + E_1. \tag{3}$$

Here, E_0 is defined as

$$\begin{aligned} E_0(x) =& 6\sum_{n=1}^{\infty}\phi(nx) + \sum_{n=1}^{\infty}\phi\left(\sqrt{\frac{p}{3}}nx\right) \\ &+ 3\sum_{n=1}^{\infty}\phi(\sqrt{3}nx) + \frac{1}{2}\sum_{n=1}^{\infty}\phi(\sqrt{p}nx), \end{aligned} \tag{4}$$

where x is taken as a variable to replace the lattice constant a. One half of the first term in Eq.(4) comes from the first summation in Eq.(2), the second term in Eq.(4) from the second summation in Eq.(2) and the third term from terms with $m = n$ of the third summation in Eq.(2). In order to match the inversion formula, we add the last term in Eq.(4). Another half of the first term is taken from the sixth and seventh summations in Eq.(2) as an approximation of their diagonal terms. E_1 in Eq.(3) is defined as the residual in Eq.(2) minus the additional term, i.e.

$$\begin{aligned} E_1 =& 3\sum_{m\neq n=1}^{\infty}\phi(\sqrt{m^2+n^2+mn}x)+6\sum_{m,n,l=1}^{\infty}\phi\left(\sqrt{m^2+n^2+mn+\frac{p}{3}l^2}x\right)+6\sum_{m,n=1}^{\infty}\phi\left(\sqrt{m^2+\frac{p}{3}n^2}x\right)\\ &+3\sum_{m,n,l=1}^{\infty}\phi\left(\sqrt{\left(m-\frac{2}{3}\right)^2+\left(n-\frac{2}{3}\right)^2+\frac{p}{3}\left(l-\frac{1}{2}\right)^2+\left(m-\frac{2}{3}\right)\left(n-\frac{2}{3}\right)}x\right)\\ &+3\sum_{m,n,l=1}^{\infty}\phi\left(\sqrt{\left(m-\frac{1}{3}\right)^2+\left(n-\frac{1}{3}\right)^2+\frac{p}{3}\left(l-\frac{1}{2}\right)^2+\left(m-\frac{1}{3}\right)\left(n-\frac{1}{3}\right)}x\right)\\ &-\left[3\sum_{n=1}^{\infty}\phi(nx)+\frac{1}{2}\sum_{n=1}^{\infty}\phi(\sqrt{p}nx)\right]. \end{aligned} \tag{5}$$

We define two operators T_0 and T_1, in terms of which E_0 and E_1 can be expressed in the pair potential ϕ

$$E_0 = T_0\phi(x), \tag{6}$$

and

$$E_1 = T_1\phi(x). \tag{7}$$

Therefore, the cohesive energy can be written as

$$\begin{aligned} E(x) =& E_0 + E_1 = (T_0+T_1)\phi\\ =& T_0(1+T_0^{-1}T_1)\phi(x). \end{aligned} \tag{8}$$

If we make an inversion operation, we can obtain the pair potential from the cohesive energy immediately

$$\phi(x) = (1+T_0^{-1}T_1)^{-1}T_0^{-1}E(x). \tag{9}$$

Expanding Eq.(9), we obtain

$$\phi(x) = (1-T_0^{-1}T_1+T_0^{-1}T_1T_0^{-1}T_1-\cdots)T_0^{-1}E(x). \tag{10}$$

This equation shows that if we want to extract the pair potential ϕ from the cohesive energy E, even when we know the definition of operator T_1 from Eqs.(5) and (7), we still need to know the operator T_0^{-1}. Making an inversion operation for Eq.(6), we can obtain an expression for operator T_0^{-1}, but it is involved with an operation inverse to the summation. Although at present there is no available mathematical theorem allowing us to solve this problem, however the Möbius theorem in the number theory might be a very useful means. This theorem states[6] that if

$$F(x) = \sum_{n=1}^{\infty} f(nx), \tag{11}$$

then

$$f(x) = \sum_{n=1}^{\infty}\mu(n)F(nx), \tag{12}$$

provided $\sum_{m,n=1}^{\infty}|f(mnx)|$ exists. $f(x)$ and $F(x)$ are real functions, and $\mu(n)$ is the so-called Möbius function, the definition of which is

$$\mu(n) = \begin{cases} 1, & \text{if } n=1,\\ (-1)^s, & \text{if } n \text{ includes } s \text{ distinct primes},\\ 0, & \text{if } n \text{ includes repeat factors}. \end{cases} \tag{13}$$

By means of the above theorem, we can prove that the operator T_0^{-1} is equal to a new operator N defined as

$$\begin{aligned} Nf(x) =& \frac{1}{6}\sum_{m,u,l=1}^{\infty}\left(-\frac{1}{6}\right)^{m-1}\left(-\frac{1}{2}\right)^{u-1}\\ &\times\mu(l)f\left[\left(\frac{p}{3}\right)^{\frac{m-1}{2}}3^{\frac{u-1}{2}}lx\right], \end{aligned} \tag{14}$$

where $f(x)$ is a real function and $\mu(l)$ is the Möbius function. This formula is called the general Möbius inversion transform formula for hcp lattices. The proof is given in the Appendix.

Based on Eq.(A7), we can rewrite Eq.(10) as

$$\phi = (1-NT_1+NT_1NT_1-\cdots)NE. \tag{15}$$

If the cohesive energy E is given, in terms of Eqs.(5), (7) and (14), we can obtain the pair potential by using Eq.(15).

4. Calculation of the phonon dispersion relations in zinc

Using the above general Möbius inversion transform formula for hcp lattices, we can obtain the interatomic interaction from the cohesive energy, and then study properties of materials with either ideal hcp structures or with non-ideal hcp structures.

In this paper we choose zinc as an example to study its phonon dispersion relations along some symmetrical directions. The structure of zinc is non-ideal and its c/a ratio is much larger than the ideal value.

The phonon dispersion relations in zinc have been studied by many authors. In earlier years, the phonon dispersions in crystals with hcp lattice were studied in tensor force models. In these models some force constants were introduced. In the absence of the knowledge of interactions between atoms, these force constants were obtained in terms of elastic constants instead of directly calculating them from interatomic interactions. Because the number of force constants is larger than that of elastic constants in tensor force models, some simplified models have appeared, such as central-force models,[7,8] A-S models,[9] non-central force models,[10,11] and so on. In these models the force constants were evaluated from elastic constants, or from phonon frequencies measured at some special points in the Brillouin zone, or from both. Another way to treat phonon dispersion relations is to use the first-principles method in some pseudo-potential models.[12−15] But the results of most of these works were unsatisfactory.

In 1993, Li *et al.*[4] proposed a method to calculate the phonon dispersion relations for fcc metals, based on a direct calculation of force constants using the interatomic interactions, which were converted from the cohesive energies by means of the Möbius inversion transform formula for fcc lattices. Here we use this method to calculate the phonon dispersion relations in zinc in terms of the general Möbius inversion transform formula mentioned above for hcp lattices.

4.1. The cohesive energy of zinc

In order to obtain the interatomic interaction between atoms in zinc by means of the general Möbius inversion transform formula, we need to know the cohesive energy of zinc, as stated above. We calculate the cohesive energy per atom in zinc by first using the linear muffin tin orbital method. It is found that the calculated results can be fitted by a Morese-type potential with proper parameters

$$E(x) = E_0(e^{-2\alpha(x-a_0)} - 2\mathrm{e}^{-\alpha(x-a_0)}), \qquad (16)$$

where E_0 is the cohesive energy and a_0 is the lattice constant, and both are due to the equilibrium configuration of the lattice. α is a decay factor. By fitting the calculated results, we obtain $E_0 = 1.366$eV/atom, a_0=2.635Å and α=1.629/Å. The corresponding experimental values for E_0 and a_0 are 1.35eV/atom and 2.66Å respectively.[1]

4.2. The pair potential between atoms in zinc

For the convenience of numerical calculation of the pair potential ϕ, we introduce some coefficients defined as follows

$$Nf(x) = \sum_{p=1}^{\infty} W'_p f(s'_p x) \qquad (17)$$

and

$$T_1 f(x) = \sum_{q=1}^{\infty} W'_q f(s'_q x), \qquad (18)$$

where N and T_1 are operators defined above, and $f(x)$ is a real function. Substituting Eqs.(17) and (18) into Eq.(15) yields

$$\begin{aligned}\phi =& \sum_{p_0}^{\infty} W'_{p_0} E(s'_{p_0} x) \\ &- \sum_{p_0,p_1,q_1}^{\infty} W'_{p_0} W'_{p_1} W'_{q_1} E(s'_{p_0} s'_{p_1} s'_{q_1} x) \\ &+ \sum_{p_0,p_1,q_1,p_2,q_2}^{\infty} W'_{p_0} W'_{p_1} W'_{p_2} W'_{q_1} W'_{q_2} \\ &\times E(s'_{p_0} s'_{p_1} s'_{p_2} s'_{q_1} s'_{q_2} x) - \cdots \\ =& \sum_{p}^{\infty} W_p E(s_p x). \end{aligned} \qquad (19)$$

The coefficients W'_p and s'_p can be calculated beforehand by use of Eq.(14), and W'_q and s'_q can be obtained by use of Eqs.(7) and (5). Then the coefficients W_p and s_p can be obtained by use of Eq.(19). It should be noted that the above coefficients are dependent on the parameter p. Therefore, they are different for different materials. Based on Eqs.(16) and (19) and the calculated coefficients W_p and s_p, we have calculated the pair potential for zinc, as shown in Fig.2.

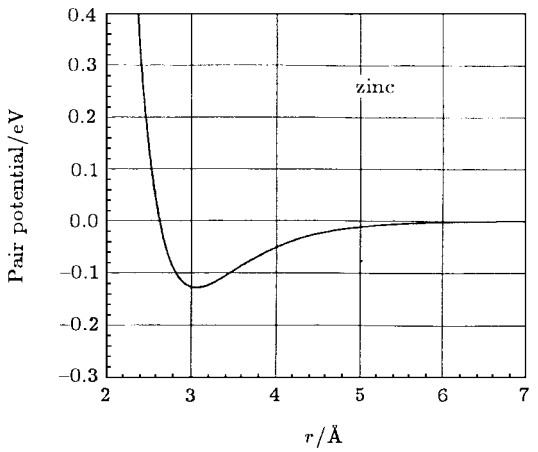


Fig.2. The calculated pair potential for zinc.

4.3. The phonon dispersion relations along some symmetrical directions in zinc

Using the calculated pair potential ϕ, we can express the total energy of zinc in terms of the positions of its atoms

$$\Phi = \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_N). \tag{20}$$

When atoms vibrate around their equilibrium positions, we can expand the total energy Φ in their displacements[16]

$$\begin{aligned}\Phi =& \Phi_0 + \sum_{m,n,\alpha}^{\infty} (\frac{\partial \Phi}{\partial u_{m,n,\alpha}})_0 u_{m,n,\alpha} \\ &+ \frac{1}{2} \sum_{m,n,\alpha,m'n'\alpha'} \left(\frac{\partial^2 \Phi}{\partial u_{m,n,\alpha} \partial u_{m',n',\alpha'}}\right)_0 \\ &\times u_{m,n,\alpha} u_{m',n',\alpha'} + \cdots,\end{aligned} \tag{21}$$

where Φ_0 is the static value of Φ in the equilibrium configuration, and $u_{m,n,\alpha}$ is the α-component of the displacement of the nth atom in the mth unit cell. The subscript "0" denotes that the values of the derivatives are taken at equilibrium positions. In a harmonic approximation, the vibration energy of a crystal is

$$\begin{aligned}\Phi' =& \frac{1}{2} \sum_{m,n,\alpha,m'n'\alpha'} \left(\frac{\partial^2 \Phi}{\partial u_{m,n,\alpha} \partial u_{m',n',\alpha'}}\right)_0 \\ &\times u_{m,n,\alpha} u_{m',n',\alpha'}.\end{aligned} \tag{22}$$

Motions of the atoms can be described by

$$\begin{aligned}M_n \ddot{u}_{m,n,\alpha} =& - \sum_{m',n',\alpha'} \left(\frac{\partial^2 \Phi}{\partial u_{m,n,\alpha} \partial u_{m',n',\alpha'}}\right)_0 \\ &\times u_{m',n',\alpha'},\end{aligned} \tag{23}$$

where M_n is the mass of the nth atom and $-\left(\frac{\partial^2 \Phi}{\partial u_{m,n,\alpha} \partial u_{m',n',\alpha'}}\right)_0$ are so-called force constants.

The frequencies of atom vibrations are given by the following secular equation[16]

$$|D_{\alpha\alpha',nn'} - \omega^2 \delta_{\alpha\alpha'} \delta_{nn'}| = 0, \tag{24}$$

where $\delta_{nn'}$ is the Kronecker delta, and $D_{\alpha\alpha',nn'}$ is an element of the so-called dynamical matrix, which is concerned with force constants.

We have directly computed the force constants by use of the calculated pair potential for zinc and then the elements of the dynamical matrix. Solving Eq.(24), we obtain the phonon dispersion relations along directions T, T', Σ and Δ (see Figs.3 and 4), but the results are unsatisfactory. As mentioned in the introduction, here we consider the effect of the three-body interaction. The Slater–Kirkwood-type three-body potential is also adopted[17]

$$\begin{aligned}\phi^{(3)}(r_i, r_j, r_{ij}) =& [A \mathrm{e}^{-p(r_i + r_j + r_{ij})} + C(r_i r_j r_{ij})^{-3}] \\ &\times (1 + 3\cos\theta_i \cos\theta_j \cos\theta_{ij}),\end{aligned} \tag{25}$$

where r_i, r_j, r_{ij} are the sides of a triangle and $\theta_i, \theta_j, \theta_{ij}$ are its interior angles respectively. A, C and p are parameters. Choosing $A = -1000.0$eV, $C = -1000.0$eV (Å)^9, and p=1.100/Å, we insert Eq.(25) into Eq.(1) and re-inverse Eq.(1) to achieve a new two-body interaction. Using the new two-body interaction and the three-body interaction, we re-compute the phonon dispersion relations. The calculated results are plotted in Fig.4 and compared with the inelastic neutron scattering data.[18]

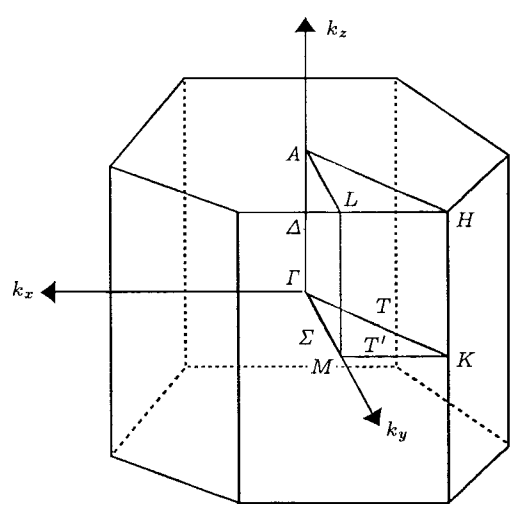


Fig.3. The first Brillouin zone of a hcp lattice.

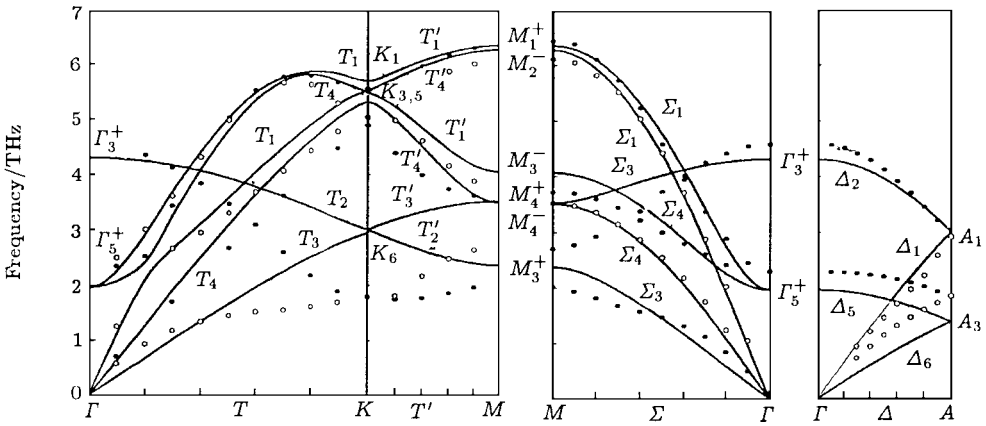


Fig.4. The phonon dispersion relations along directions T, T', Σ and Δ. The solid lines denote the calculated values in the present work, and the open and filled circles represent the experimental data measured by the inelastic neutron scattering.[18]

5. Discussion

The obtained Möbius inversion transform formula can be applied to all materials with hcp structures and with any value of the ratio c/a. If we have obtained the cohesive energy E either from *ab initio* calculation or from semi-empirical fitting, we can calculate the two-body interaction between atoms in materials with hcp structures by use of the present method and then study their properties in terms of the calculated two-body interactions. Generally speaking, the interaction among atoms in materials is complex. The pair potential is a first-order approximation. In this frame, it not only allows us to obtain the two-body interaction, but also allows us to consider the effect of many-body interactions, as in the present work for zinc. The present method does not include any adjustable parameters and essentially it is based on the first-principles calculation. This method presents a useful means to study the properties of hcp-structured materials in the interatomic force model. Especially, we can use the obtained interatomic interaction to study properties of some complex systems in this model.

We choose zinc as our example, because it is a typical material with a non-ideal hcp structure. The value of its c/a ratio deviates obviously from the ideal one. The phonon dispersion relations have been measured[18−20] and studied by many authors as cited above. In previous works, some authors achieved some poor results and went so far as to obtain imaginary frequencies. Others obtained good results, but had to use some adjustable parameters, which seemed to be unreasonable.[13] Many authors have pointed out that there was an obvious anisotropy in zinc[7,15,18] and the three-body interaction was employed by some authors to study the lattice dynamics of metals with hcp structure.[21] In our calculations the results also show that a three-body interaction is needed to acquire acceptable results of the phonon dispersion relations in zinc. This is attributed to the strong anisotropy in this metal. From Fig.4, the obvious discrepancies are found for T_2, T_2', T_3 and T_3' near the zone boundary K. They might be caused by the fact that we only consider the contribution from nearest neighbours through third nearest neighbours to the force constants, and the contribution from next nearest neighbours was ignored.

6. Appendix

From Eq.(6) we have

$$NT_0\phi(x) = NE_0(x). \tag{A1}$$

In terms of Eq.(4) and Eq.(14), we can express Eq.(A1) as

$$\begin{aligned} NT_0\phi(x) =& N\sum_{n=1}^{\infty}\Big[6\phi(nx) + \phi\Big(\sqrt{\frac{p}{3}}nx\Big) \\ &+ 3\phi(\sqrt{3}nx\Big) + \frac{1}{2}\phi(\sqrt{p}nx)\Big] \\ =& \sum_{m,n,l,u=1}^{\infty}\Big\{\Big(-\frac{1}{6}\Big)^{m-1}\Big(-\frac{1}{2}\Big)^{u-1} \\ &\times \mu(l)\phi\Big[\Big(\frac{p}{3}\Big)^{\frac{m-1}{2}}3^{\frac{u-1}{2}}lnx\Big] \\ &-\Big(-\frac{1}{6}\Big)^{m}\Big(-\frac{1}{2}\Big)^{u-1}\mu(l)\phi\Big[\Big(\frac{p}{3}\Big)^{\frac{m}{2}}3^{\frac{u-1}{2}}lnx] \\ &-\Big(-\frac{1}{6}\Big)^{m-1}\Big(-\frac{1}{2}\Big)^{u}\mu(l)\phi\Big[\Big(\frac{p}{3}\Big)^{\frac{m-1}{2}}3^{\frac{u}{2}}lnx\Big] \\ &+\Big(-\frac{1}{6}\Big)^{m}\Big(-\frac{1}{2}\Big)^{u}\mu(l)\phi\Big[\Big(\frac{p}{3}\Big)^{\frac{m}{2}}3^{\frac{u}{2}}lnx\Big]\Big\}. \end{aligned} \tag{A2}$$

If we let $m' = m - 1$, Eq.(A2) becomes

$$
\begin{aligned}
NT_0\phi(x) = & \sum_{m'=0,n,l,u=1}^{\infty} \left(-\frac{1}{6}\right)^{m'} \left(-\frac{1}{2}\right)^{u-1} \\
& \times \mu(l)\phi\left[\left(\frac{p}{3}\right)^{\frac{m'}{2}} 3^{\frac{u-1}{2}} lnx\right] \\
& - \sum_{m,n,l,u=1}^{\infty} \left(-\frac{1}{6}\right)^{m} \left(-\frac{1}{2}\right)^{u-1} \\
& \times \mu(l)\phi\left[\left(\frac{p}{3}\right)^{\frac{m}{2}} 3^{\frac{u-1}{2}} lnx\right] \\
& - \sum_{m'=0,n,l,u=1}^{\infty} \left(-\frac{1}{6}\right)^{m'} \left(-\frac{1}{2}\right)^{u} \\
& \times \mu(l)\phi\left[\left(\frac{p}{3}\right)^{\frac{m'}{2}} 3^{\frac{u}{2}} lnx\right] \\
& + \sum_{m,n,l,u=1}^{\infty} \left(-\frac{1}{6}\right)^{m} \left(-\frac{1}{2}\right)^{u} \\
& \times \mu(l)\phi\left[\left(\frac{p}{3}\right)^{\frac{m}{2}} 3^{\frac{u}{2}} lnx\right] \\
= & \sum_{n,l,u=1}^{\infty} \left(-\frac{1}{2}\right)^{u-1} \\
& \times \mu(l)\phi(3^{\frac{u-1}{2}} lnx) - \sum_{n,l,u=1}^{\infty} \left(-\frac{1}{2}\right)^{u} \\
& \times \mu(l)\phi(3^{\frac{u}{2}} lnx). \qquad \text{(A3)}
\end{aligned}
$$

Letting $u' = u - 1$, Eq.(A3) can be expressed as

$$
\begin{aligned}
NT_0\phi(x) = & \sum_{n,l=1,u'=0}^{\infty} \left(-\frac{1}{2}\right)^{u'} \mu(l)\phi(3^{\frac{u'}{2}} lnx) \\
& - \sum_{n,l,u=1}^{\infty} \left(-\frac{1}{2}\right)^{u} \mu(l)\phi(3^{\frac{u}{2}} lnx) \\
= & \sum_{l,n=1}^{\infty} \mu(l)\phi(lnx). \qquad \text{(A4)}
\end{aligned}
$$

From Eqs.(11) and (12) we can deduce

$$
\begin{aligned}
f(x) &= \sum_{l=1}^{\infty} \mu(l)F(lx) \\
&= \sum_{l=1}^{\infty} \mu(l) \sum_{n=1}^{\infty} f(nlx) \\
&= \sum_{l,n=1}^{\infty} \mu(l) f(lnx) \qquad \text{(A5)}
\end{aligned}
$$

Comparing Eqs.(A4) and (A5), we conclude that

$$NT_0 = I, \qquad \text{(A6)}$$

where I is the unit operator. Therefore, we have

$$T_0^{-1} = N. \qquad \text{(A7)}$$

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