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Modified mean-field potential approach to thermodynamic properties of a low-symmetry crystal: Beryllium as a prototype

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We extend the mean-field potential (MFP) approach for evaluating the vibrational contribution of the lattice ion of high-symmetry metals, and present a modified MFP approach which can be applied to low-symmetry or complex structure crystals. Based on the modified MFP approach in which the effect of the structural parameters on the free energy is taken into account, a first-principles scheme for calculating thermodynamic properties of a crystal dependent on the crystal structure is developed. By taking hexagonal close-packed beryllium as a prototype, we demonstrate that our scheme is suitable for investigating the structural properties and equation of state of low-symmetry crystals.

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I. INTRODUCTION

Interest in *ab initio* (without empirical parameters) calculations of the equation of state and relative stability of crystal structures has been high for many years. First-principles electronic-structure methods are routinely used to compute the zero-temperature internal energy but can also be used to calculate the Helmholtz free-energy contributions from the ions and the electrons, which results in a complete equation of state. The contribution from the electrons can usually be obtained from the first-principles band structures. However, the contribution from the ions is difficult to calculate accurately because the volume and temperature dependence of the phonon frequencies and the density of state are complicated.

At present, there are several ways to examine the lattice vibrational contribution without using empirical parameters. The first uses the Debye model and may incorporate a volume dependence of the Debye temperature calculated using the first-principles-based methods.[1,2] The Debye model is quick and easy but explicitly works out anharmonic contributions which is very important at high temperature. The second is the linear-response lattice dynamics. First-principles linear-response calculations can give important lattice dynamics information, but it is computationally expensive. Additionally, it usually requires the use of the quasiharmonic approximation, and anharmonic effects are usually neglected. The third is molecular dynamics. It is even more computationally expensive to study the thermal equation of state properties rigorously from first-principles molecular-dynamics calculations directly. Molecular dynamics usually requires small system sizes and neglects quantum occupation of phonon states.

The fourth is a certain mean-field approximation, including the particle-in-a-cell (PIC) model[3,4] and the so-called mean-field potential approach proposed by Wang *et al.*[5–9] The PIC model assumes that each atom is confined to the Weigner-Seitz cell formed by its nearest neighbors. Although interatomic correlations are neglected and, as has been implemented are, classical, the PIC model includes anharmonic terms which are important for high temperatures. Calculations using this model usually are performed on supercells of several hundreds of atoms for the different lattices with periodic boundary conditions.[10,11] Because the PIC calculation is also very time consuming and inconvenient, Wang *et al.* proposed a classical analytic mean-field potential (MFP) approach. The MFP approach has been demonstrated to match successfully the thermal properties of various metals. It is worth noting that the metals calculated in the work of Wang *et al.* have a high symmetry, for example, Al, Cu, and Ce with a fcc structure, and Ta, Mo, and W with a bcc structure.[5–7] For low-symmetry metals, such as bct-Th and bct-U, the axial ratio c/a is fixed, without considering the influence of c/a varying with volume.[8]

In this paper, we extend the MFP approach to more general cases where the effect of the structural parameters varying with volume on the total free energy is taken into account, and present a modified MFP approach which can be applied to low-symmetry or complex structure crystals. Based on the modified MFP approach a first-principles scheme for calculating thermal properties of a crystal dependent on the crystal structure is developed. Taking hexagonal close-packed (hcp) beryllium (Be) as a prototype, we demonstrate that our scheme correctly describes most of the structural and thermodynamic properties.

The rest of this paper is organized as follows. In Sec. II, we present the general theory of the modified MFP approach. In Sec. III taking hcp Be as a prototype, we present our calculated structural and thermodynamic properties, and compare those with the experimental data. The results are encouraging. Finally, our summary is given in Sec. VI.

II. MODIFIED MFP APPROACH

The modified MFP approach is based on the MFP model and expends it to more general cases where the effect of the structural parameters varying with volume on the total free energy is taken into account, so that the modified MFP approach can be presented for low-symmetry or complex structure crystals. For a crystal with a given temperature T and a given averaged atomic volume V that is a function of the structural parameters $\{a_i\}$, the Helmholtz free energy $F[V(\{a_i\}),T]$ per ion can be written as

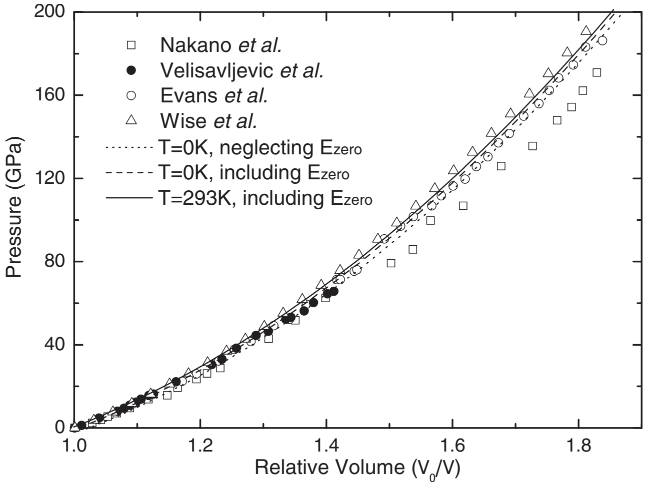

FIG. 1. Theoretical 0 and 293 K isothermal equations of state of hcp Be compared with room-temperature experimental data: Open squares, Nakano *et al.* (Ref. 21); filled circles, Velisavljevic *et al.* (Ref. 22); open circles, Evans *et al.* (Ref. 23), and open triangles are the room-temperature isotherm derived from experimental shock-wave data of Wise *et al.* (Ref. 35). The solid line represents 293 K isotherm considering zero-point energy correction E_{zero}. The dotted and dashed lines correspond to 0 K isotherms neglecting and including E_{zero}, respectively. V_0 is the atomic volume under ambient conditions, 8.11 Å^3.

$$F[V(\{a_i\}),T] = E_c[V(\{a_i\})] + F_{el}[V(\{a_i\}),T] + F_{ion}[V(\{a_i\}),T], \tag{1}$$

where $E_c[V(\{a_i\})]$ is the zero-temperature classical energy, i.e., the ground-state energy when the ions are fixed at their lattice sites, $F_{el}[V(\{a_i\}),T]$ is the thermal free energy from electronic excitations, and $F_{ion}[V(\{a_i\}),T]$ is the vibrational contribution to the free energy.

The zero-temperature classical energy $E_c[V(\{a_i\})]$ can be calculated using density-functional theory[12,13] within the generalized-gradient approximation. The electronic contribution to the free energy $F_{el}=E_{el}-TS_{el}$ depends on the electronic density of states as a function of volume, $n[\epsilon, V(\{a_i\})]$. The occupation of these states given by the Fermi distribution f determines the electronic entropy[14]

$$S_{el}[V(\{a_i\}),T] = -k_B \int n[\epsilon, V(\{a_i\})] \times [f \ln f - (1-f)\ln(1-f)] d\epsilon, \tag{2}$$

where k_B is Boltzmann's constant. The energy E_{el} due to the electron excitations can be expressed as

$$E_{el}[V(\{a_i\}),T] = \int n[\epsilon, V(\{a_i\})] f \epsilon d\epsilon - \int^{\epsilon_F} n[\epsilon, V(\{a_i\})] \epsilon d\epsilon, \tag{3}$$

where ϵ_F is the Fermi energy.

The vibrational contribution to the free energy F_{ion} can be formulated as

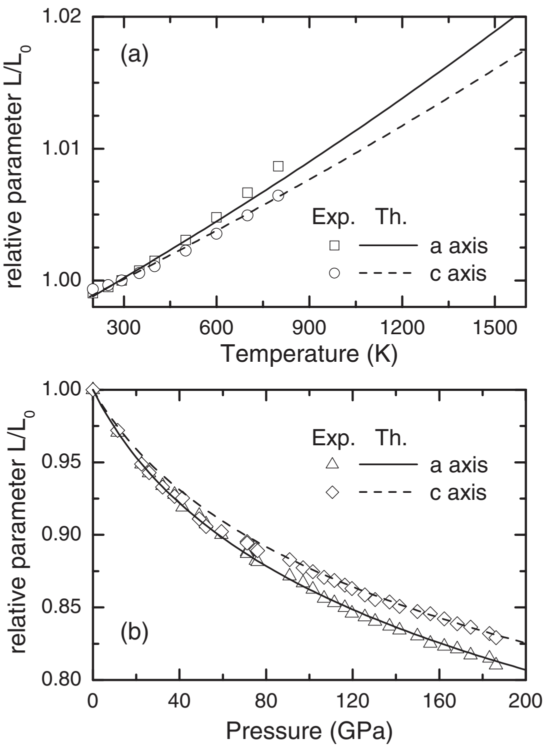

FIG. 2. (a) Calculated relative lattice parameters of hcp Be, L/L_0 ($L=a,c$), as a function of temperature at ambient pressure. Open squares and circles represent experimental data from Ref. 39. (b) Calculated lattice parameters as a function of pressure at room temperature. Open triangles and diamonds represent experimental data from Ref. 23. L_0 ($L=a,c$) is lattice parameters of hcp Be under ambient conditions.

$$F_{ion}[V(\{a_i\}),T] = -k_BT\left\{\frac{3}{2}\ln\frac{mk_BT}{2\pi\hbar^2} + \ln v_f[V(\{a_i\}),T]\right\}, \tag{4}$$

where

$$v_f[V(\{a_i\}),T] = 4\pi \int \exp\left\{-\frac{g[r,V(\{a_i\})]}{k_BT}\right\} r^2 dr, \tag{5}$$

$\hbar$ is Planck's constant, and m is the mass of each ion. $g[r,V(\{a_i\})]$ in Eq. (5) is the MFP, and the central issue of the mean-field theory is how to calculate the MFP $g[r,V(\{a_i\})]$. In this paper, we take the following form proposed by Wang *et al.*:[5–9]

$$g[r,V(\{a_i\})] = \frac{1}{2}[E_c(R+r) + E_c(R-r) - 2E_c(R)], \tag{6}$$

where R is the nearest distance between atoms and r corresponds to the distance of a single atom displaced from its equilibrium position. Notice that $g[r,V(\{a_i\})]$ depends on all the structural parameters $\{a_i\}$.

The equilibrium structure of the crystal at any T and V can be determined by minimizing the Helmholtz free energy

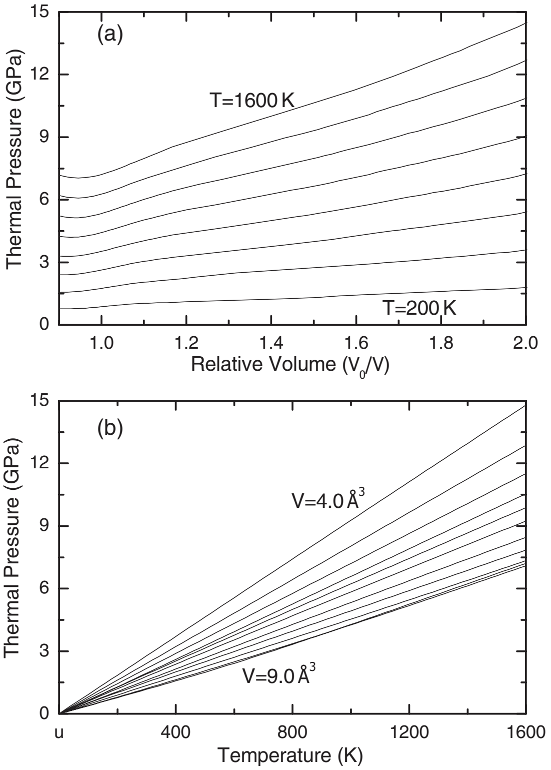

FIG. 3. Thermal pressure of hcp Be (a) as a function of relative volume for temperatures from 200 up to 1600 K with 200 K interval and (b) as a function of temperature for volumes varying from 4.0 to 9.0 Å^3/atom with 0.5 Å^3/atom interval. V_0 is the atomic volume under ambient conditions, 8.11 Å^3.

$$F[V(\{a_i\}),T] = E_c[V(\{a_i\})] + F_{el}[V(\{a_i\}),T] + F_{ion}[V(\{a_i\}),T] \tag{7}$$

with respect to all the structural parameters $\{a_i\}$. Once the minimal Helmholtz free energy $F(V,T)$ at a given T and V is known, namely, the free energy corresponding to the equilibrium structure at a given T and V, other thermodynamic functions and the thermal properties of the crystal can be deduced. For example, internal energy $E(V,T)$, pressure $P(V,T)$, and the isothermal bulk modulus $B_T(V,T)$ can be, respectively, calculated as

$$E(V,T) = F(V,T) - T\left[\frac{\partial F(V,T)}{\partial T}\right]_V, \tag{8}$$

$$P(V,T) = -\left[\frac{\partial F(V,T)}{\partial V}\right]_T, \tag{9}$$

$$B_T(V,T) = V\left[\frac{\partial^2 F(V,T)}{\partial V^2}\right]_T. \tag{10}$$

III. EXAMPLE: HCP BERYLLIUM

To illustrate the application of the modified MFP approach we have described, we investigate the equation of state and the structural properties of hcp Be, which has a low-symmetry structure and for which some related experimental data are available. We compare our calculational results with the available experimental data and the other theoretical results, and demonstrate that our scheme correctly describes most of the structural and thermodynamic properties.

Be has stimulated much experimental and theoretical research interest because of its simple atomic electronic configuration and unusual physical properties. At ambient conditions, Be crystal has a hcp structure with the axial ratio $c/a=1.568$ that significantly differs from the ideal value of 1.633.[15,16] This nonideal behavior is ascribed to the highly anisotropic bonding properties.[17,18] Unusually high Debye temperature (1440 K) and very small Poisson's ratio (0.05) of hcp Be suggest that the behavior of valence electrons deviates substantially from that of near free electrons.[17] Be shows very interesting and complex behavior under different temperature and pressure conditions. At ambient pressure and high temperature, Be crystal transforms from a hcp structure to a body-centered-cubic (bcc) structure at 1523 K and melts at 1551 K.[19] At elevated pressure (up to 6 GPa) and high temperature, the hcp-bcc phase boundary has a negative slope, and the transition temperature decreases with increasing pressure.[20] While at ambient temperature and high pressure, recent x-ray-diffraction studies have found no hcp-bcc transition at pressures approaching 200 GPa.[21–23]

Because Be has very high Debye temperature, the contribution of zero-point vibrations to Be thermodynamic functions is expected to be more important than in other systems and cannot be ignored. Then, we modify the expression of Eq. (1) and replace E_c by E_0 $(=E_c+E_{zero})$, where E_{zero} is the energy of zero-point vibrations. E_0 includes the zero-temperature classical energy E_c and the contributions of zero-point vibrations E_{zero}, and hence it represents the static zero-temperature total energy of the system. Correspondingly, the Helmholtz free energy and the mean-field potential related to E_0 can be written as

$$F[V(\{a_i\}),T] = E_0[V(\{a_i\})] + F_{el}[V(\{a_i\}),T] + F_{ion}[V(\{a_i\}),T] \tag{11}$$

and

$$g[r,V(\{a_i\})] = \frac{1}{2}[E_0(R+r) + E_0(R-r) - 2E_0(R)]. \tag{12}$$

E_{zero} can be obtained from the Debye model

$$E_{zero}(V) = \frac{9}{8}k_B\Theta(V), \tag{13}$$

where $\Theta(V)$ is a volume dependence of the Debye temperature reported in Ref. 24.

For hcp Be, the crystal structural parameters are a and c axes. In fact, at a given V and T, for the determination of Helmholtz free energy of the hcp structure, it is enough to minimize the function $F[V(\{a_i\}),T]=F(V,c/a,T)$ with respect to only one variable, namely, the c/a ratio.

TABLE I. Comparison of experimental and calculated atomic volumes V_0, lattice parameters a and c, axial ratio c/a, isothermal bulk modulus B_0, and pressure derivative of bulk modulus B_0' for hcp Be under ambient pressure.

	T=293 K Expt.	T=0 K neglecting E_{zero}	T=0 K including E_{zero}	T=293 K including E_{zero}
V_0 (Å^3/atom)	8.105,[a] 8.110[b]	7.924	8.053	8.145
a (Å)	2.285,[a] 2.286[b]	2.265	2.278	2.287
c (Å)	3.585,[a] 3.584[b]	3.566	3.584	3.595
c/a	1.569,[a] 1.568[b]	1.574	1.573	1.572
B_0 (GPa)	110,[c] 114,[d] 117,[e] 118,[f] 119[g]	122	118	116
B_0'	3.59,[c] 3.52,[f] 3.48[g]	3.46	3.47	3.45

[a] From Ref. 15, static.
[b] From Ref. 16, static.
[c] From Ref. 23, static.
[d] From Ref. 33, static.
[e] From Ref. 34, static.
[f] From Ref. 35, shock.
[g] From Ref. 36, shock.

A. Static equation of state

We first discuss the static zero-temperature high-pressure properties of hcp Be. The ground-state energy calculations are performed using the Vienna *ab initio* simulation package,[25,26] which is based on the density-functional theory. Exchange and correlation functional is given by the generalized-gradient approximation of PBE form.[27] Electron-ion interaction is represented by the projector-augmented wave (PAW) method,[28] as implemented by Kresse and Joubert.[29] The PAW method is an all-electron technique similar to other standard implementations such as full-potential linear augmented plane waves,[30] as well as being closely related to the ultrasoft pseudopotential method.[31] We test kinetic-energy cutoff and k-point sampling to assure a total-energy convergence of 1 meV per atom. As a result of the convergence tests, the kinetic-energy cutoff is 400 eV for all calculations, and the k-point meshes of Brillouin-zone sampling based on the Monkhorst-Pack scheme[32] are $31\times31\times31$.

The calculated zero-temperature properties of hcp Be under ambient pressure are compared with experiment in Table I. It is found that the energy of zero-point vibrations E_{zero} plays an important role in determining the zero-temperature properties of hcp Be and further improves the agreement with experimental data. The contribution of zero-point vibrations expands the atomic volume 2%, results in a 0.6% increase in both lattice parameters, and causes the isothermal bulk modulus to decrease by 3%. The static calculations neglecting and including E_{zero} at $T=0$ K give $a=2.265$ Å, $c/a=1.574$ and $a=2.278$ Å, $c/a=1.573$, respectively, to be compared with the experimental values $a=2.286$ Å, $c/a=1.568$, which also agree with the theoretical results from Debye model[24,37] and quasiharmonic approximation calculations.[38]

Because the pressure contribution from the electron excitations and lattice vibrations at ambient temperature is small (see Sec. III B), the calculated equation of state at zero temperature is compared directly with room-temperature data, as shown in Fig. 1. It is found that the calculated isotherms are in agreement with data from static[22,23] and shock[35] experiments, and the isotherm including E_{zero} is more accurate than that neglecting E_{zero}. The isotherms satisfactorily agree with the experimental data[21] up to 70 GPa, however, progressively disagrees for higher pressures. It is clearly shown that our theoretical results and experimental data[22,23,35] are substantially stiffer than that of Nakano *et al.*[21] The difference between these static experiments may be caused by the following. Evans *et al.*[23] used a hydrostatic medium, helium, in order to avoid systematic effects in determining the pressure in a nonhydrostatic sample with a pressure gradient. Velisavljevic *et al.*[22] also employed copper as a pressure marker and medium. However, Nakano *et al.*[23] used no medium, and their results may be better if considering the corrections to the ruby pressure scale, as proposed in Ref. 24. From the discussion above, it can be seen that the experimental data in Refs. 22, 23, and 35 are more reliable and agree well with our theoretical results.

B. Thermal equation of state and structural properties

As mentioned above, we evaluate the Helmholtz free energies at different volumes and temperatures by a direct minimization over the c/a ratio of the free energy $F(V,c/a,T)$. From the resulting free energies, we calculate some hcp Be parameters under ambient conditions and summarize them in Table I. The agreement with the experimental values is excellent when the zero-point vibrations and thermal expansivity are added to our theoretical predictions.

To further evaluate the accuracy of our calculations, we plot the relative lattice parameters of hcp Be, L/L_0 ($L=a,c$), as a function of temperature at ambient pressure in Fig. 2(a) and as a function of pressure at room temperature in Fig. 2(b), in comparison with experimental data. It can be seen that the calculated results are in good agreement with experimental data,[23,39] which indicates that the calculation

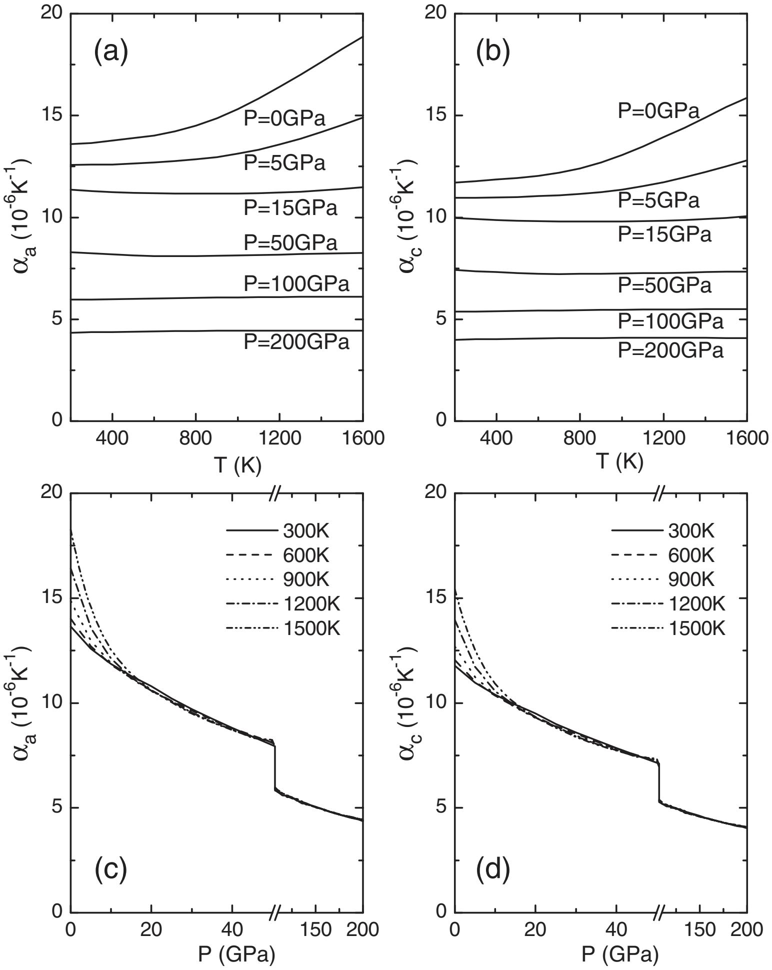

FIG. 4. The linear thermal-expansion coefficients of hcp Be as functions of temperature [(a) for *a* axis and (b) for *c* axis] and pressure [(c) for *a* axis and (d) for *c* axis].

accounts well for Be bulk anisotropic changes in the temperature and pressure range of interest. At ambient pressure, the lattice parameters increase slowly with increasing temperature, and the thermal expansion of the *a* axis is slightly larger than that of the *c* axis; while at room temperature, the lattice parameters decrease continuously with increasing pressure, and the *a* axis is more compressible than the *c* axis.

In Fig. 1, we also plot the 293 K isothermal equation of state of hcp Be including E_{zero}. The 293 K isotherm is very close to zero-temperature isotherm, which indicates that the pressure contribution from the electron excitations and lattice vibrations at room temperature is small. It is also clearly seen that our calculated 293 K isotherm exactly goes through more reliable data from static[22,23] and shock[35] experiments as mentioned above. Furthermore, we compare our isotherm with the theoretical results from Debye model[24,37] and find that they agree well with each other.[40]

The thermal pressure can be obtained from the pressure difference between isotherms. The thermal pressures as a function of relative volume V_0/V are shown in Fig. 3(a). At low temperature, the thermal pressures are small and show little volume dependence. At elevated temperature, the magnitude of thermal pressure increases significantly, and their values first show a little decrease with increase of relative volume, and then show an increase for relative volumes larger than 0.95. The thermal pressures as a function of temperature are shown in Fig. 3(b). At a given volume, the thermal pressure shows a linear increase with temperature. Moreover, the thermal pressure shows a strong volume dependence. This is different from bcc Ta, where the thermal pressure has a slope of ~0.004 42 GPa/K for almost all the volumes.[11] The different thermal pressure behaviors of hcp Be might be partly due to the effect of the structural parameters varying with volume.

The thermal properties related to the lattice parameters are the linear thermal-expansion coefficients. Knowing the lattice parameters of hcp Be, *a* and *c* axes, at a given *T* and *P* as shown in Fig. 2, one can obtain the linear thermal-expansion coefficients by definition

$$\alpha_a = \frac{1}{a}\left(\frac{\partial a}{\partial T}\right)_P, \tag{14}$$

$$\alpha_c = \frac{1}{c}\left(\frac{\partial c}{\partial T}\right)_P. \tag{15}$$

In Fig. 4, we plot the calculated linear thermal-expansion coefficients of hcp Be as functions of temperature and pressure. It is clearly shown that at the same *T* and *P*, α_a is larger than α_c. α_a and α_c at ambient conditions are, respectively, equal to 14×10^{-6}/K and 12×10^{-6}/K, which agree with the experimental data of 12×10^{-6}/K and 10×10^{-6}/K.[41] The linear thermal-expansion coefficients are very sensitive parameters. At low pressures, α_a and α_c show a clear increase

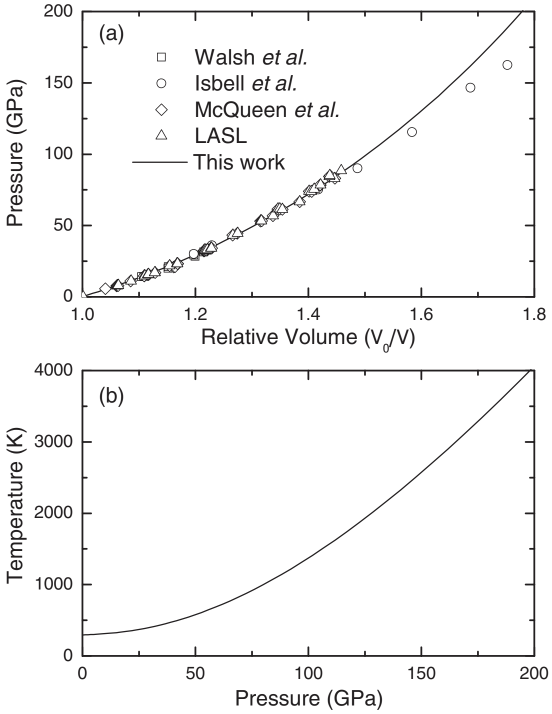

FIG. 5. (a) Theoretical Hugoniot for hcp Be (solid line) compared with experimental Hugoniot data: Open squares, Walsh *et al.* (Ref. 42); open circles, Isbell *et al.* (Ref. 43); open diamonds, McQueen *et al.* (Ref. 44); and open triangles, LASL (Ref. 45). V_0 is the atomic volume under ambient conditions, 8.11 Å^3. (b) Theoretical temperatures along the Hugoniot.

with temperature; at moderate pressures, α_a and α_c first decrease slowly with increase of temperature, and then increase slowly for temperatures larger than ~800 K; while at high pressures, α_a and α_c are almost independent of temperature [Fig. 4(a)]. On the other hand, the calculated thermal-expansion coefficients show a rapid drop with increasing pressure [Fig. 4(b)].

The only source of information on the equation of state of hcp Be at high compression and high temperatures is shock-wave data. From shock-wave data which are characterized by shock velocity D and particle velocity u, one can define Hugoniot states with $V_H/V_0=(D-u)/D$ and $P_H=\rho_0 Du$, where P_H and V_H are the final pressure and volume, and V_0 and ρ_0 are the initial volume and density. To compare our results of the equation of state of hcp Be at high compression and high temperatures with those derived from the shock-wave data, we calculated the pressures P_H and temperatures T_H on the Hugoniot of hcp Be by solving the Rankine-Hugoniot equation

$$P_H(V_0-V_H)=2(E_H-E_0), \qquad (16)$$

where E_H is the internal energy along the Hugoniot, and V_0 and E_0 are the atomic volume and internal energy at ambient conditions, respectively. For a given volume V, the temperature T_H on the Hugoniot is varied until Eq. (16) is satisfied. At pressures below 88 GPa, the calculated Hugoniot shows an excellent agreement with the shock-wave experimental measurements[42–45] [Fig. 5(a)] and other theoretical results of Robert and Sollier[37] who calculate pressure only up to 100 GPa. However, for pressures above 92 GPa, the discrepancy between our Hugoniot and experimental data is clear and may be attributed to hcp-bcc phase transition in metal Be. To check up this assumption, we compute the temperatures along the Hugoniot in Fig. 5(b) and compare it with the hcp-bcc phase coexistence curve calculated by Sin'ko *et al.*[24] We find the two curves across at about 90 GPa and 1180 K, the pressure in the range between 88 and 92 GPa. This indicates that our assumption is reasonable. The detailed discussion about the hcp-bcc phase transition and the multiphase equation of state for Be will be in the later work.

IV. SUMMARY

In this paper, we develop the MFP model proposed by Wang *et al.* to more general cases where the effect of the structural parameters varying with volume on the total free energy is taken into account, and present a modified MFP approach which can be applied to low-symmetry or complex structure crystals.

Based on the modified MFP approach, we present a first-principles scheme to calculate thermodynamic properties of a crystal dependent on its structure. By taking hcp Be as a prototype, we investigate the crystal properties at ambient conditions, lattice parameters varying with temperature and pressure, thermal equation of state, and Hugoniot curve, which show a good agreement with available experimental data and other theoretical results. These demonstrate that our scheme correctly describes most of the structural and thermodynamic properties of low-symmetry metals.

The present modified MFP approach is not just limited to the case of low-symmetry metal but also applied to other complex systems with the quasimonatomic crystal types, such as NaCl and BeO. Because our scheme depends on the crystal structures and permits efficient computation, it can be used to calculate the vibrational free energy of these crystal structures, and then used to construct a multiphase equation of state.

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