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Analytic Debye-Grüneisen equation of state for a generalized Lennard-Jones solids*

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The approximate method to treat the practical quantum anharmonic solids proposed by Hardy, Lacks and Shukla is reformulated with explicit physical meanings. It is shown that the quantum effect is important at low temperature, it can be treated in the harmonic framework; and the anharmonic effect is important at high temperature and tends to zero at low temperature, it can be treated by using a classical approximation. The alternative formulation is easier for various applications, and is applied to a Debye-Grüneisen solid with the generalized Lennard-Jones intermolecular interaction. The expressions for the Debye temperature and Grüneisen parameter as a function of volume are analytically derived. The analytic equation of state is applied to predict the thermodynamic properties of solid xenon at normal-pressure with the nearest-neighbour Lennard-Jones interaction, and is further applied to research the properties of solid xenon and krypton at high pressure by using an all-neighbour Lennard-Jones interaction. The theoretical results are in agreement with the experiments.

Keywords: equation of state, analyticity, generalized Lennard-Jones solid, thermodynamic properties
PACC: 6250, 6400

1. Introduction

In recent years, many semi-empirical equation of state (EOS) for solids have been proposed.[1−12] However, a simple and accurate molecular thermodynamic EOS reliable over the whole temperature range is not yet available even for the simplest molecular solids. The most commonly used Debye-Grüneisen (DG) EOS is also semi-empirical. Most of the DG-type EOS has assumed that both Debye temperature and Grüneisen parameter are constants independent of volume and temperature, but many experiments and theories have shown that both quantities should be volume dependent.[9,10] The assumption thus results in a semi-empirical EOS.

The semi-empirical EOS has several typical drawbacks. First of all, these EOS always deal with the cold and hot pressures separately, a cold EOS is firstly proposed, and some semi-empirical methods are used to further consider the hot pressure. It is obviously impossible to establish a reliable self-consistent EOS theory by using such a method. The second problem is that these EOS must introduce some semi-empirical parameters with little or no physical meaning, which are usually determined by fitting the thermodynamic properties in certain temperature and density ranges, so the extension of the corresponding EOS to other temperature and density ranges is in doubt. The third is that these EOS do not take many important effects into account, such as the correlation effect at low temperature and anharmonic effect at high temperature. Westera and others[12−16] have shown that the correlation effect is small, its negligence may not cause severe problem; however, the anharmonic effect is very important at high temperature, its negligence may result in serious problems.[17,18]

In order to improve the DG-type EOS, many authors devoted to establishing the function of the Grüneisen parameter as the volume.[9,10] Yet most of these functions are not based on the intermolecular interaction and are semi-empirical. Otherwise, the harmonic or lowest anharmonic approximations are generally used in the molecular thermodynamic works

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for the solids.[19−26] However, Shukla and co-workers have shown that the anharmonic expansion for solid is slowly convergent at low temperature or divergent at slightly high temperature.[27,28] So the anharmonic effects must be carefully treated at high temperature.

Several years ago, Hardy, Lacks and Shukla (HLS) proposed an approximate method to treat the anharmonic and quantum effects at the same time.[29] The main point of the method is to expand the free energy of a practical solid as an infinite anharmonic series. Although the classical expansion is divergent, the quantum modifications for all anharmonic terms are absolutely convergent. One can add these quantum modifications to a classical free energy expression and only consider the lower few terms. Hardy *et al*, firstly used the method to modify a classical molecular dynamic (MD) simulation, the obtained results are in good agreement with the more complicated effective-potential Monte Carlo (EPMC) and path integral Monte Carlo (PIMC) simulations. However, after Hardy *et al* works using the method are scarce. The reason may be that the HLS method is firstly proposed for a classical molecular dynamic simulation, yet it is difficult to obtain the quantum modifications in the MD simulation. But an analytic EOS with some approximation, such as the DG-type EOS, is favourable in practice and people have not been aware of the strength of the method for improving these analytic EOS.

In this work, we reformulate the HLS method with explicit physical meaning, and use the method to research a generalized Lennard-Jones (GLJ) solid. In section 2, the method is reformulated, and the relationship of DG EOS with intermolecular interaction is generally derived. In section 3, the general formalism is applied to a GLJ solid. In section 4, the analytic EOS is applied to solid xenon and krypton. At last, the conclusion is given in section 5.

2.Relationship of DG EOS with intermolecular interaction

As the practical solid must be an anharmonic quantum crystal, we write the partition function Z as $Z_{\rm aq}$, and reformulate it as

$$Z \equiv Z_{\rm aq} = Z_{\rm hq}\frac{Z_{\rm aq}}{Z_{\rm hq}} = QZ_{\rm hq}, \tag{1}$$

where $Z_{\rm hq}$ is the partition function for the harmonic crystal, and Q is the quantum anharmonic factor defined as follows:

$$Q = \frac{Z_{\rm aq}}{Z_{\rm hq}}. \tag{2}$$

Considering the anharmonic effect is remarkable only at high temperature, and tends to zero at low temperature, we replace the quantum anharmonic factor in Eq.(2) by the following classical anharmonic factor:

$$Q \approx Q_{\rm cl} = \frac{Z_{\rm ac}}{Z_{\rm hc}}. \tag{3}$$

Substituting Eq.(3) into Eq.(1), the partition function Z can be approximately expressed as

$$Z \approx Q_{\rm cl}Z_{\rm hq} = Z_{\rm hq}\frac{Z_{\rm ac}}{Z_{\rm hc}}. \tag{4}$$

By using the thermodynamic relationship, $F = -kT\ln Z$, the corresponding free energy of a system can be approximately expressed as

$$F \approx F_{\rm hq} + F_{\rm am}, \tag{5}$$

$$F_{\rm am} = F_{\rm ac} - F_{\rm hc}. \tag{6}$$

Eq. (4) combined with Eq.(5) is just our reformulation. Here $F_{\rm hq}$ and $F_{\rm hc}$ are the free energies for the quantum and classical harmonic crystals respectively, $F_{\rm ac}$ is the free energy for the classical anharmonic crystal, and $F_{\rm am}$ is the classical anharmonic modification to the free energy. The physical explanation of Eq.(5) is that the free energy of a system can be approximately expressed as the sum of two parts. The first part is the free energy of a quantum harmonic crystal, the second is the classical anharmonic modification. Equation (5) can be reformulated as the equivalent form

$$F \approx F_{\rm ac} + F_{\rm qm}, \tag{7}$$

$$F_{\rm qm} = F_{\rm hq} - F_{\rm hc}, \tag{8}$$

where $F_{\rm qm}$ is the quantum modification to the free energy for a harmonic crystal. Equation (7) is the form given by Hardy *et al*.[29] Although Eq.(7) is equivalent to Eq.(5), it is more convenient to use Eq.(4) or Eq.(5), especially in the development of analytic theory with some approximations.

Now we apply the method to a DG solid. For simplicity, we start from a cell model. The fundamental assumption of the cell model is that all molecules of a system are moving in a potential field formed by other atoms symmetrically arranged around; this is essentially an Einstein model, and is also equivalent to the average field approximation. It is well known that the average field approximation gives very good results for most physical problems except the critical phenomena. Since the solid problem is far from

the critical point, the cell model indeed gives good results.[11−14]

In terms of the cell model, the average Hamiltonian of an atom takes the form[13−16]

$$H = \frac{1}{2}u(0) + \frac{\boldsymbol{p}^2}{2\mu} + [u(\boldsymbol{r}) - u(0)], \tag{9}$$

where μ is the mass of an atom, $u(\boldsymbol{r})$ is the potential energy for an atom. If adopting two-body potential, the potential energy $u(\boldsymbol{r})$ can be expressed as

$$u(\boldsymbol{r}) = \sum_{i\neq 0} \varepsilon(|\boldsymbol{R}_i - \boldsymbol{r}|) \tag{10}$$

and

$$u(0) = \sum_{i\neq 0} \varepsilon(|R_i|), \tag{11}$$

where $\varepsilon(R)$ is the two-body potential function, $\boldsymbol{R}_i$ is the position vector of the i-th atom, and $\boldsymbol{r}$ is the instantaneous displacement of the atom at the centre of a Wigner–Seitz cell. The term i=0 is excluded from the sum.

The potential energy $u(\boldsymbol{r})$ can be expanded as a series of displacement[30]

$$\begin{aligned} u(\boldsymbol{r}) - u(0) =& \frac{1}{2}(\boldsymbol{r}\cdot\nabla)^2 u(\boldsymbol{r})|_0 + \frac{1}{3!}(\boldsymbol{r}\cdot\nabla)^3 u(\boldsymbol{r})|_0 \\ &+ \frac{1}{4!}(\boldsymbol{r}\cdot\nabla)^4 u(\boldsymbol{r})|_0 + \cdots \\ =& \frac{1}{2}\nabla_r^2 u(r)|_0 \cdot r^2 + \frac{1}{3!}\nabla_r^3 u(r)|_0 \cdot r^3 \\ &+ \frac{1}{4!}\nabla_r^4 u(r)|_0 \cdot r^4 + \cdots \end{aligned} \tag{12}$$

In the development of a classical DG EOS, we have shown that the expansion is absolutely convergent,[30] one can retain only several lower terms in Eq.(12), and we only retain fourth-order term in the following derivations. In order to simplify Eq.(12), we suppose $s = |\boldsymbol{R}_i - \boldsymbol{r}|$, then we have $\mathrm{d}s = \mathrm{d}r\cos\theta$, and

$$\nabla_r^n u(r) = \sum_{i\neq 0} \cos^n\theta \cdot \nabla_s^n \varepsilon(s), \quad (n = 2, 3, 4, \cdots). \tag{13}$$

Here θ is angle of $\boldsymbol{R}_i$ and $\boldsymbol{r}$. Since $u(\boldsymbol{r})$ is highly symmetric around the centre of cell, we take average for solid angle, $\frac{1}{4\pi}\int\langle\cdots\rangle\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi$, then Eq.(13) is changed as

$$\begin{aligned} \nabla_r^n u(r) =& \frac{1}{n+1}\sum_{i\neq 0}\nabla_s^n\varepsilon(s) \\ =& \frac{1}{n+1}\sum_{i\neq 0}\left[\frac{\partial^2}{\partial s^2} + \frac{2}{s}\frac{\partial}{\partial s}\right]^{n/2}\varepsilon(s), \\ & (n = 2, 4, 6, \cdots). \end{aligned} \tag{14}$$

The terms with odd value of n equals zero after average for solid angle, and the harmonic term is in agreement with the result of Westera and Cowley.[13] It should be pointed out that the derivation of Eq.(14) from Eq.(13) is exact for cubic lattices for its cubic symmetries; one can derive out Eq.(14) directly from Eq.(13) without taking the average for solid angle. Only as Eq.(14) is used to the non-cubic lattices, such derivation becomes an approximation of spherical symmetry.

From Eq.(12), we can easily obtain the Einstein temperature

$$\Theta_{\mathrm{E}} = \frac{\hbar\omega}{k} = \frac{\hbar}{k}\left[\frac{1}{\mu}\nabla_r^2 u(\boldsymbol{r})|_0\right]^{1/2}.$$

In terms of Ref.[4], the Debye characteristic temperature Θ_{D}, and thus F_{hq} can be expressed as

$$\Theta_{\mathrm{D}} = \frac{4}{3}\Theta_{\mathrm{E}} = \frac{4\hbar}{3k_{\mathrm{B}}}\left[\frac{1}{\mu}\nabla_r^2 u(\boldsymbol{r})|_0\right]^{1/2}, \tag{15}$$

$$F_{\mathrm{hq}} = \frac{1}{2}u(0) + 9k_{\mathrm{B}}T\left(\frac{T}{\Theta_{\mathrm{D}}}\right)^3\int_0^{\Theta_{\mathrm{D}}/T} x^2\ln(1-\mathrm{e}^{-x})\mathrm{d}x. \tag{16}$$

Substituting Eq.(12) into Eq.(3), the anharmonic modification for the free energy of an atom is expressed as

$$F_{\mathrm{am}} = -k_{\mathrm{B}}T\ln Q_0, \tag{17}$$

where

$$Q_k = \frac{4}{\sqrt{\pi}}\int_0^\infty \exp(-x^2 - \lambda x^4)x^{2k+2}\mathrm{d}x, \quad (k = 0, 1, 2\cdots). \tag{18}$$

$$\lambda = \frac{k_{\mathrm{B}}T}{6}\frac{\nabla_r^4 u(r)|_0}{[\nabla_r^2 u(r)|_0]^2}. \tag{19}$$

3. Analytic equation of state for the anharmonic GLJ solid

Now we apply the formalism in previous section to the GLJ solid. The GLJ potential takes the following form:

$$\varepsilon(r) = \frac{\varepsilon_0}{m-n}\left[n\left(\frac{r^*}{r}\right)^m - m\left(\frac{r^*}{r}\right)^n\right]. \tag{20}$$

Extending the method in Ref.[30], the expressions for $u(0)$ and $\nabla_r^{2k}u(r)|_0$ $(k = 1, 2)$ can be solved as follows:

$$\nabla_r^{2k}u(r)|_0 = \frac{(2k)!\Lambda^*}{(2k+1)a^{2k}}(C_k y^{-m} - D_k y^{-n}), \quad (k = 0, 1, 2). \tag{21}$$

Here $u(0) = \nabla_r^0 u(r)|_0$, a is the distance between the nearest neighbours, and

$$\Lambda^* = z\varepsilon_0, \quad y = \left(\frac{V}{V^*}\right)^{1/3}, \tag{22}$$

$$V^* = (r^*)^3/\gamma_0, \quad V = a^3/\gamma_0, \tag{23}$$

$$\begin{aligned} C_0 =& \frac{ns_m}{m-n}, \\ D_0 =& \frac{ms_n}{m-n}, \\ C_k =& \frac{(2k+m-2)(2k+m-3)s_{m+2k}}{(2k)(2k-1)s_{m+2k-2}}C_{k-1}, \\ D_k =& \frac{(2k+n-2)(2k+n-3)s_{n+2k}}{(2k)(2k-1)s_{n+2k-2}}D_{k-1}, \end{aligned} \tag{24}$$

where z, γ_0, s_m and s_n are structural constants.[30]

Substituting Eq.(17) into Eqs.(13) and (14) leads to

$$\lambda = \frac{9}{5}\frac{k_{\mathrm{B}}T}{\Lambda^*}\frac{(C_2y^{-m} - D_2y^{-n})}{(C_1y^{-m} - D_1y^{-n})^2}, \tag{25}$$

$$\Theta_{\mathrm{D}} = \frac{4\hbar}{3k_{\mathrm{B}}r^*y}\left(\frac{2\Lambda^*}{3\mu}\right)^{1/2}(C_1y^{-m} - D_1y^{-n})^{1/2}. \tag{26}$$

The EOS can be derived analytically as

$$\xi = \frac{PV}{k_{\mathrm{B}}T} = \xi_0 + \xi_1 + \xi_2 \equiv \frac{P_0V}{k_{\mathrm{B}}T} + \frac{P_1V}{k_{\mathrm{B}}T} + \frac{P_2V}{k_{\mathrm{B}}T}, \tag{27}$$

where the three terms are cold pressure, Debye-Grüneisen and anharmonic terms, respectively.

$$\xi_0 = \frac{P_0V}{k_{\mathrm{B}}T} = \frac{\Lambda^*}{6k_{\mathrm{B}}T}(mC_0y^{-m} - nD_0y^{-n}); \tag{28}$$

$$\xi_1 = \frac{P_1V}{k_{\mathrm{B}}T} = 9\gamma_{\mathrm{G}}\left(\frac{T}{\Theta_{\mathrm{D}}}\right)^3\int_0^{\Theta_{\mathrm{D}}/T}\frac{x^3}{\mathrm{e}^x - 1}\mathrm{d}x, \tag{29}$$

where γ_{G} is the Grüneisen parameter,

$$\begin{aligned} \gamma_{\mathrm{G}} =& -\frac{V}{\Theta_{\mathrm{D}}}\frac{\partial\Theta_{\mathrm{D}}}{\partial V} \\ =& \frac{[(m+2)C_1y^{-m} - (n+2)D_1y^{-n}]}{6(C_1y^{-m} - D_1y^{-n})}; \end{aligned} \tag{30}$$

$$\xi_2 = \frac{P_2V}{k_{\mathrm{B}}T} = \frac{\eta\lambda Q_2}{3Q_0}, \tag{31}$$

where η is an auxiliary quantity introduced here

$$\begin{aligned} \eta =& -\frac{y}{\lambda}\frac{\partial\lambda}{\partial y} = \frac{(mC_2y^{-m} - nD_2y^{-n})}{(C_2y^{-m} - D_2y^{-n})} \\ & - \frac{2(mC_1y^{-m} - nD_1y^{-n})}{(C_1y^{-m} - D_1y^{-n})}. \end{aligned} \tag{32}$$

For the convenience of determining potential parameters, we derived the following relationship from Eq.(28):

$$\Lambda^* = \frac{18y^3V^*}{\beta_P^0}(m^2C_0y^{-m} - n^2D_0y^{-n})^{-1}, \tag{33}$$

where β_P^0 is the isothermal compressibility coefficient at zero temperature.

4. Numerical results for solid xenon and krypton

The parameters for the nearest-neighbour LJ model of solid xenon have been given in literature.[13] In order to check our EOS, we firstly use these parameters to research the thermodynamic properties for the solid xenon at normal pressure. The results are shown in Fig.1. The results under harmonic approximation and the experimental data[13] for the solid xenon are also given in this figure. The reduced units ($\varepsilon_0 = r^* = k = 1$) is used with the value of parameters appropriate to a nearest-neighbour interaction of xenon. For the thermal expansion and heat capacity at constant volume, three sets of experimental points are shown. These are based on three different measurements of the thermal expansion.[31−33]

Figure 1 shows that the results including the anharmonic effects is in good agreement with the experiments; the results for the harmonic approximation is in agreement with the experiments only at low temperature, at slightly high temperature the results becomes divergent; however, the results with and without the anharmonic effects are in agreement with each other at low temperature. These results show that the anharmonic effect is very important at high temperature, and indeed tends to zero at low temperature, so its classical treatment is reasonable.

The experimental data of thermal expansivity from Tilford and Swenson[31] have slightly larger values. However, Tilford and Swenson have pointed out that one of the three sets of experimental data has a systematic error; if it is the set with small values, we can see from Fig.1 that our theoretical results are in agreement with the experimental data with large values at an acceptable precision. One of other possible reasons is that the LJ potential is only applicable to the gaseous rare gases, but for the solid rare gases it becomes unrealistic. For example, Barker *et al* have used a modified form of the Barker-Pompe potential for two-body interactions and have included the Axilrod-Teller triple-dipole interaction in a perturbation calculation.[17−19] The calculated thermodynamic properties at very low temperature are in good agreement with the experimental data of Tilford and Swenson.[31−33]

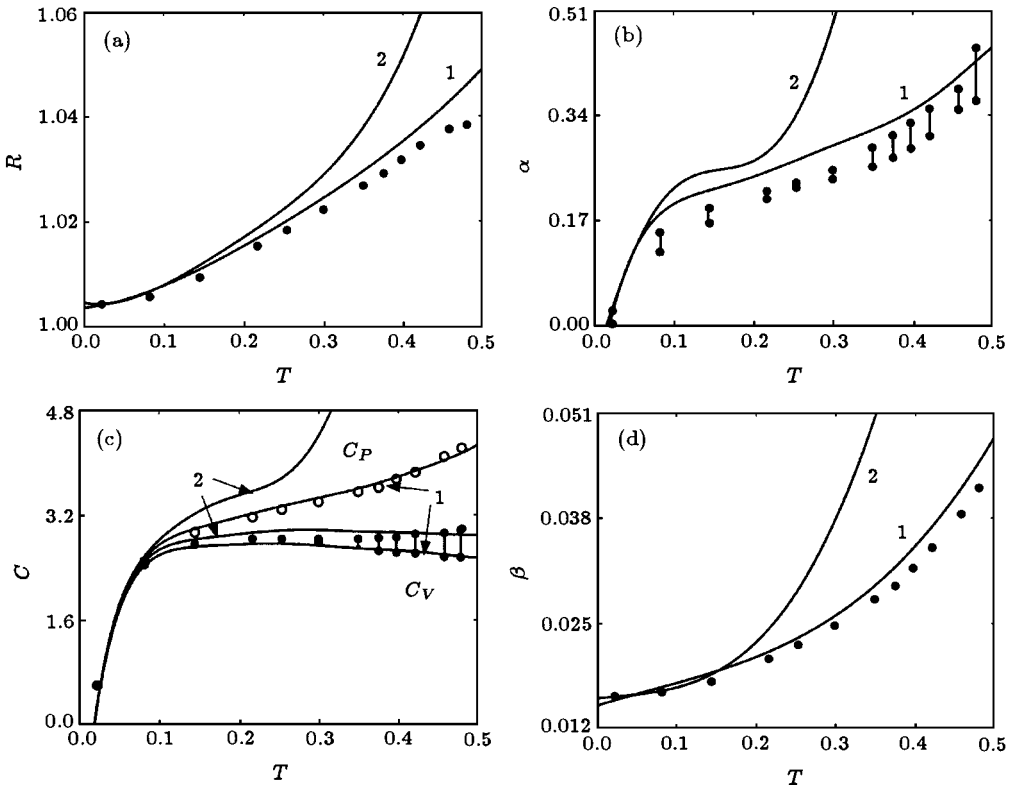


Fig.1. Thermodynamic properties for the solid xenon, in reduced units for the nearest-neighbour Lennard-Jones potential: solid lines, theoretical; symbols, experimental. Curve 1 is anharmonic; curve 2 is harmonic. (a) Nearest-neighbour distance; (b) volume thermal expansivity; (c) heat capacity at normal pressure, three sets of experimental values for C_V are derived from the C_P curve using different values for the thermal expansivity; (d) isothermal compressibility.

Although the nearest-neighbour LJ model gives fairly well results for the properties of solid xenon at normal pressure, the model cannot well describe the compression curves of rare solids at high pressure. So we further use an all-neighbour GLJ model to research the compression curves of rare solids at high pressure. In all-neighbour GLJ model, we find that the potential parameter n can be taken as a constant n=6, and other three parameters m, ε_0 and r_e for solid krypton and xenon are determined by fitting the experimental data of β_P^0, atomic volume V and isothermal expansivity coefficient α_T at some temperature and at normal pressure. The experimental data[18] and the solved parameters are listed in Tables 1 and 2, respectively.

Using these value of parameters determined by using the properties at normal pressure, we predict the compression curves for solid xenon and krypton at high pressure. Figure 2 shows that the predicted compression curves are in good agreement with the experiments. By using the same parameters we also calculated the thermal expansivity and isothermal compressibility coefficients versus temperature, the agreement of theoretical results with experiment are as good as the nearest-neighbour LJ model, which, for clarity, is not given here.

Table 1. Experimental data used to determine the potential parameters.

Material	μ	V/nm^3	$\alpha_T/10^6\mathrm{K}^{-1}$	$\beta_P/10^{11}\mathrm{m}^2\cdot\mathrm{N}^{-1}$
Kr	83.8	0.04582	756	29.67
Xe	131.3	0.05902	615	27.45

Note. The experimental data of β_P are at 0 K and are taken from Ref.[18], the others for Kr are at 40 K, for Xe are at 60 K and are taken from Ref.[19].

Table 2. Calculated values of parameters for the LJm-6 potential.

Material	m	n	r_e/nm	$\frac{\varepsilon_0}{k}\Big/\mathrm{K}$
Kr	11.43	6	0.41219	165.85
Xe	11.08	6	0.44805	233.89

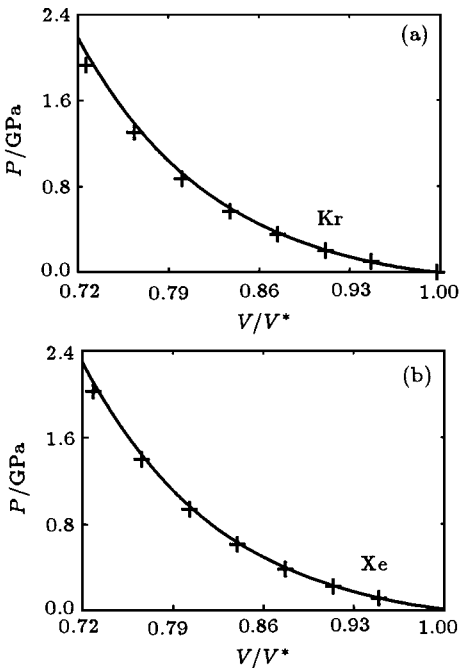


Fig.2. Comparison of experimental and predicted compression curves. (a) Kr, (b) Xe. The experimental data (+) are taken from Ref.[18].

It has been recognized that the Debye model gives good description of thermodynamic properties of solids at low temperature within the harmonic framework. Combining the reformulated HLS method used in this paper to consider the anharmonic effects, we think this is a practically acceptable approach for the research of thermal properties of practical solids.

5. Conclusion

In summary, we reformulated Hardy *et al*'s method to treat the quantum and anharmonic effects separately. The physical explanation of the reformulation is that the quantum effect only is important at low temperature, and in that case, the atoms of lattice are vibrating as harmonic oscillators, so the quantum effect is treated under the harmonic frame. The anharmonic effect is important at high temperature where the classical theory is applicable; at low temperature it tends to zero, so the effect is treated under the classical approximation. The potential energy of an atom is expanded as an absolutely convergent series of displacement; this makes the treatment of anharmonic effect more convenient. The method can completely take the anharmonic effect into account and include important part of the quantum effect, and can be easily extended to other potentials to develop practical molecular thermodynamic EOS for solids.

The reformulated method is used to develop the molecular thermodynamic theory for an anharmonic generalized Lennard-Jones solid. The potential energy for an atom is expanded as absolutely convergent series of radial coordination to consider the anharmonic effect. Combining the Debye model to consider the quantum effect, we derived the analytic equation of state. The results including anharmonic effect are in good agreement with the experiments, and that without anharmonic effect is divergent at high temperature. The consideration of anharmonic effect is shown being very important at high temperature.

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