

How accurate for phonon models to predict the thermodynamics properties of crystals

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Abstract

Previous work has shown that thermodynamics properties calculated by phonon model with quasi-harmonic approximation (QHA) may differ badly from experiment in some cases. The inaccuracy was examined in the present work by comparing the results of QHA for argon and copper crystal with the ones of molecular dynamics simulations, partition functions obtained by a new method or experiment. It is shown that QHA works well for the systems of atomic volume smaller than $22 \text{ \AA}^3/\text{atom}$ and the accuracy gets lower and lower gradually with increasing of the atomic volume. Based on this fact, the disagreement (or agreement) between the thermodynamics properties of MgO, Si, CaO, ZrO₂ calculated in previous work by QHA and the experiments can be well understood.

Keywords: phonon model, quasi-harmonic approximation, statistical physics

(Some figures may appear in colour only in the online journal)

1. Introduction

Theoretical evaluations of the thermal properties of crystalline materials have vast applications, such as in alloy design, service analysis or the phase transition at high pressure and high temperature [1, 2], and can be realized in principle by calculating the partition function (PF) formulated in statistical mechanics without empirical parameters. However, the accurate solution to PF of condensed matter has been a problem since the birth of statistic mechanics, and even at the present, it is yet difficult to gain the PF via *ab initio* calculations for realistic systems [3]. On the other hand, the phonon model based on harmonic approximation provides a possible route to compute the free energy (or PF) of crystals, and has been applied in many aspects via quasi-harmonic approximation

(QHA) accounting a variety of thermal properties of crystalline materials [4]. Based on the fact that the displacements of crystal atoms from the equilibrium lattice sites are generally small compared to inter-atomic distance, QHA would work well for lower temperatures but not for high temperatures. Indeed, the calculated specific heat (C_V) of Si crystal below 300 K is in excellent agreement with the experiment and deviates gradually from experiment as the temperature increasing [5]. At 800 K, the difference is about 10% and the agreement deteriorates at higher temperatures. It is surprising that the calculations of MgO crystal up to 2000 K coincide very well with experiment [6], while similar procedure performed for CaO by two of the four authors, however, produced quite unsatisfactory results [7]. The calculated thermal expansion coefficient for B1 structure (NaCl structure) of CaO at room temperatures differs from the experimental value by 17%, and the difference is much larger than 35% above 1000 K. Similar calculations

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of ZrO₂ showed that the theoretical isotherm bulk modulus at 300 K is about 25% lower than the experimental value and the difference gets larger above 1000 K though the agreement of volume expansion, molar specific heat (C_P) and entropy is fair in a temperature zone up to 1000 K or higher [8].

The above mentioned disagreement (or agreement) may be caused by the shortcomings of QHA model or by the inaccurate calculations of the phonon dispersion that depend heavily upon various algorithms for addressing the many-electron interaction. For the B1 structure of CaO crystal [7], as an example, phonon dispersion calculated by DFT coincides well with the experimental observation, but the calculated thermal expansion coefficient is significantly small and the author denied that the discrepancy stems from the local-density approximation employed instead of the generalized gradient approximation. Based on this fact together with the general considerations of theoretical physics, it is highly desired to carefully examine the accuracy of QHA for thermal property predictions under specific conditions. Thanks to modern computer techniques, molecular dynamics simulation (MD) can be performed vastly to test QHA in details because the same interaction potential between the atoms can be employed in both QHA and MD, and therefore the difference between MD and QHA inevitably reveals the accuracy of QHA. Of course, other theoretical approaches to the thermal properties of condensed matter are also desired to test QHA. A direct integral approach (DIA) developed very recently is a good choice since its high accuracy and efficiency have been demonstrated by several systems, such as condensed copper using tight-binding (T-B) potential [3], graphene and γ -graphyne materials using Brenner potential [9] and solid argon using Lennard–Jones (L–J) potential [10].

In the present work, we first demonstrated that quantum effect in crystals would disappear when the DeBroglie wavelength of the atoms is significantly smaller than their size, indicating that classical MD simulations can reproduce experimental result, such as internal energy and equation of state under common experimental conditions (relatively higher temperatures), and then the method together with DIA was applied to examine the accuracy of QHA for argon and copper crystals with the atomic volume changed from 11 to 40 Å³/atom. It is shown that the accuracy of QHA depends mainly on the atomic volume, which can well explain why the calculations for MgO by QHA are excellent but quite unsatisfactory for CaO.

2. Models and methods

2.1. MD simulation

Although quantum MD simulation is a reasonable way to test QHA, it needs too much computational costs for a system consisting of more than hundreds of atoms. Relatively, the cost of classical MD simulation is much smaller while quantum effects of crystal atoms fully included in QHA are excluded in classical MD. Actually, the quantum effects would disappear under common experimental conditions. According to previous work [11], when the DeBroglie wavelength of particles is much shorter than their size, the classical mechanics can

produce the same results as quantum mechanics. For an atom in a condensed state at temperature T , the DeBroglie wave length is expressed by $\lambda_T = \left(\frac{h^2}{2\pi mkT}\right)^{\frac{1}{2}}$, which is smaller than the atomic size (~ 2 Å) when T is above 100 K except for H or He atom. For argon atoms, λ_T decreases from 0.28 Å down to 0.16 Å when temperature increases from 100 to 300 K. Thus, it can be expected that the quantum effect of atomistic motion in crystal will get weaker and weaker as the temperature increasing and classical MD can reproduce experimental results when the temperature is above 100 K. This conclusion was confirmed by the following example.

Considering that the interaction potential between argon atoms in solids can be well modeled by pairwise L–J function [12, 13], we performed classical MD simulations of argon crystals to produce the pressure along the melting line, which was compared with experimental measurement [14] to see dependencies of the relative difference upon the DeBroglie wavelength of the thermal atoms. Specifically, the systems consisting of 1372 atoms were arranged in fcc structure with a lattice constant of 5.256 Å in a cubic box with periodic boundary conditions (PBC), and the interaction potential was taken as [13],

$$\phi(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^6 \right], \quad (1)$$

where r_{ij} is the distance between atoms i and j , $\epsilon = 117.05$ (K), $\sigma = 3.4$ Å and the cutoff distance is 12.0 Å. The simulations were performed by the Large-scale Atomic/Molecular Massively Parallel Simulator software package [15] with a time step of 0.1 fs and the Nose–Hoover constant-temperature algorithm [16] was used to produce a canonical ensemble at temperature T . The system was allowed to relax for 20 ps at first and then continued to run for another 80 ps, during which averages of pressure obtained by the virial theorem [17, 18] were recorded in every 10 fs.

The pressures obtained from the MD and experiment [14] are shown in figure 1(a). At a roughly glance, (seeing the inset of figure 1(a)), the agreement between the simulation and experiment is good for temperatures above 100 K, while further analysis shows that the relative difference decreases from 23.22% to 1.27% as the temperature increasing from 100 up to 300 K (figure 1(a)). Now that the L–J potential can reproduce the experimental data with high precision at higher temperatures, we have no sufficient argument to say that the potential gets inaccurate for lower temperatures. Then, what causes the larger discrepancy at lower temperatures? The answer should be the quantum effects of the thermal motion of atoms since the λ_T increases from 0.15 Å for 320 K up to 0.28 Å for 100 K.

The above example suggests that when λ_T is shorter than 0.23 Å, the deviation of the classical MD due to ignoring quantum effects can be reduced down to smaller than 5%. This conclusion should be universal for other atom or molecule (except for H and He atom) crystals since the atom's size is nearly the same, ~ 2 Å, and is applicable to the following classical MD simulations.

In the classical MD simulations of copper crystals (section 3), the interaction between atoms is described by the

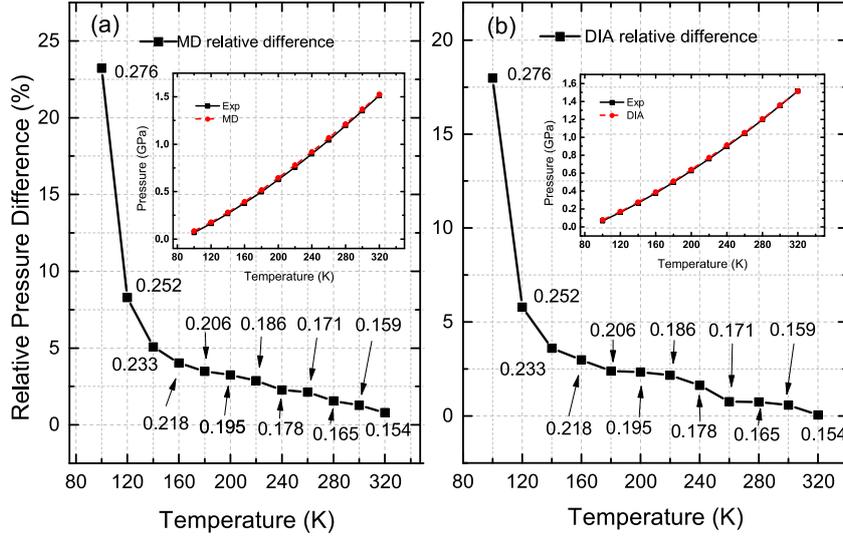


Figure 1. For the argon crystal along the melting line, the relative difference of pressure between the experiment [14] and MD simulations (a), or DIA calculations (b). The numbers along the curve denote λ_T for each temperature and the insets display the pressure values.

T-B potential [19], which has been successfully applied to determine the phase diagram of silicon [20, 21], and the total potential energy for N-atom is expressed by

$$U = \sum_i^N (E_B^i + E_R^i), \quad (2)$$

with

$$E_B^i = - \left\{ \sum_j \xi^2 e^{-2q(r_{ij}/r_0-1)} \right\}^{1/2}, \quad (3)$$

and

$$E_R^i = \sum_j A e^{-p(r_{ij}/r_0-1)}, \quad (4)$$

where constants A , ξ , p , q , r_0 and a_0 equal to 0.0855 eV, 1.224 eV, 10.960, 2.278, 2.557 Å and 3.615 Å, respectively. Obviously, this is a many-body interaction potential rather than the pair-wise two-body potential for argon system. The MD procedures for this system are nearly the same as for the argon crystal except that the virial theorem for counting the pressure was not adopted because it is only accurate for two-body interaction potential with PBC applied. For the copper system, we employed the method proposed by Tsai [22] applicable to arbitrary potential form with PBC applied for doing the statistic of pressure via considering the stress and momentum flux across a plane.

2.2. Direct integral approach

DIA to solutions of PF is applicable to calculations of thermal properties of both liquid and solid [3]. For a canonical ensemble consisting of N particles confined in volume V at temperature T , the PF reads

$$\mathcal{Z}(N, V, T) = \left(\frac{2\pi m}{h^2 \beta} \right)^{\frac{3N}{2}} Q(q^{3N}), \quad (5)$$

where h , m and β are the plank constant, the atomic mass and $(k_B T)^{-1}$, respectively. Setting $Q^{3N} = \{Q_1, Q_2, \dots, Q_{3N}\}$ the coordinates of particles with a spatial configuration of the lowest potential energy U_0 , we introduce relative coordinates $q^{3N}(q'_1, q'_2, \dots, q'_{3N})$ by $q'_i = q_i - Q_i$ to define a relative potential by

$$U'(q^{3N}) = U(q^{3N}) - U_0. \quad (6)$$

By inserting equation (6) into equation (5), we obtain

$$Q = e^{-\beta U_0} \int dq^{3N} \exp[-\beta U'(q^{3N})], \quad (7)$$

which can be solved as

$$Q = e^{-\beta U_0} \prod_{i=1}^{3N} \mathcal{L}_i, \quad (8)$$

where \mathcal{L}_i represents the effective length on the i th degree of freedom and is defined by

$$\mathcal{L}_i = \int e^{-\beta U'(0, \dots, q'_i, \dots, 0)} dq'_i. \quad (9)$$

For homogeneous systems with certain geometric symmetry, such as perfect one-component crystals, all the particles are equivalent and U' felt by one particle moving along q'_x may be the same as the one along q'_y (or q'_z). In such a case, equation (8) turns into

$$Q = e^{-\beta U_0} \mathcal{L}^{3N}, \quad (10)$$

where \mathcal{L} is determined by equation (9). Otherwise, it is needed to calculate the effective length, \mathcal{L}_x , \mathcal{L}_y , \mathcal{L}_z respectively, and equation (8) turns into

$$Q = e^{-\beta U_0} (\mathcal{L}_x \mathcal{L}_y \mathcal{L}_z)^N, \quad (11)$$

and, E and P are thus evaluated as

$$E = \frac{3}{2} N k_B T + U_0 + 3N \frac{\sum_{i=1}^n U_i \exp[-\beta U_i]}{\sum_{i=1}^n \exp[-\beta U_i]}, \quad (12)$$

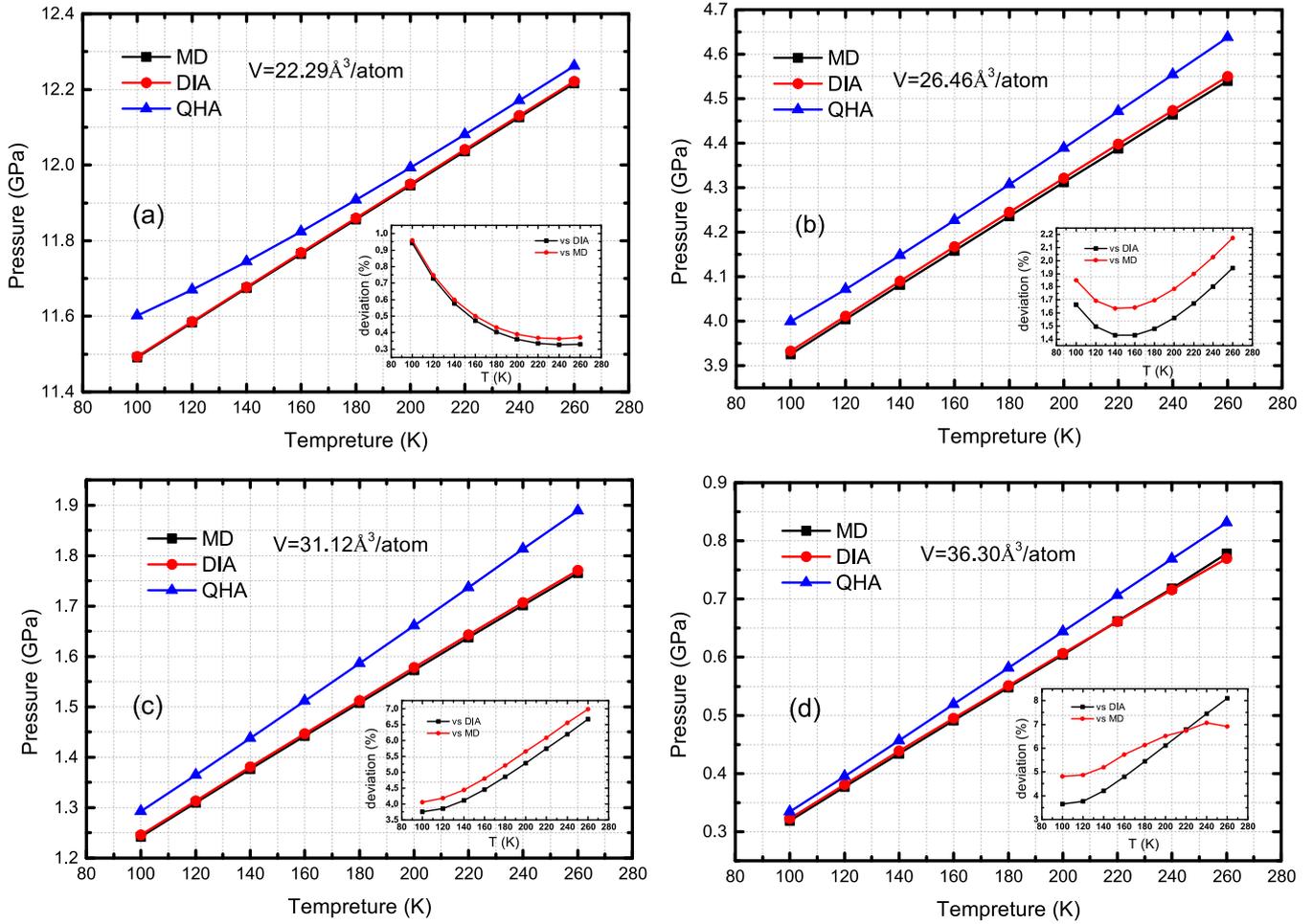


Figure 2. Pressure of 1372 argon atoms in the solid state obtained by DIA (red circles), QHA (blue triangles) and MD simulations (black squares) with the atomic volume of $22.29 \text{ \AA}^3/\text{atom}$ (a), $26.46 \text{ \AA}^3/\text{atom}$ (b), $31.12 \text{ \AA}^3/\text{atom}$ (c) and $36.30 \text{ \AA}^3/\text{atom}$ (d) at different temperatures. The insets illustrate the relative difference between QHA and MD or DIA. The error bars of MD simulations are too small to be shown in the figure.

$$P \approx - \frac{U_0(V + \Delta V) - U_0(V)}{\Delta V} + \frac{3N}{\beta} \frac{1}{\mathcal{L}(V)} \frac{\mathcal{L}(V + \Delta V) - \mathcal{L}(V)}{\Delta V}. \quad (13)$$

It should be pointed out that the quantum effect of atomistic motion is not included in DIA because the expression of PF (equation (5)) is based on classical mechanics. Thus, similar to the MD simulations discussed in the last subsection, DIA can not work well at lower temperatures. As an example, DIA was performed on the same argon system as the one of last subsection. Specifically, the atoms were placed right at the fcc sites to produce U_0 , and $U'(0, \dots, q'_i, \dots, 0)$ in equation (9) was obtained by moving the center atoms along its Z-axis ([100] direction) step by step with an interval of 0.001 \AA to record the potential via equation (1) for 2×10^4 times, during which the coordinates of its X-axis, Y-axis, and Z-axis of all the other particles were kept fixed. The pressure was calculated by equation (13) with a volume difference ($\Delta V/V$) of 10^{-15} , corresponding to length of the cubic box changed by 10^{-5} . As shown in figure 1(b), the pressures obtained from DIA above 100 K coincide well with those of experimental

measurements while it works worse at 100 K, which is similar to the performance of MD simulations (figure 1(a)).

2.3. Phonon calculations

For a crystal in equilibrium state at temperature T , the atoms (or ions) vibrate with displacement $\mu(ij)$ around the lattice sites $\mathbf{r}(ij)$, where i and j are the labels of unit cells and atoms in each unit cell, respectively, and the total potential can be expanded as

$$\begin{aligned} \Phi &= \Phi_0 + \sum_{ij} \sum_{\alpha} \Phi_{\alpha}(ij) \mu_{\alpha}(ij) \\ &+ \frac{1}{2} \sum_{i'i', j'j'} \sum_{\alpha\beta} \Phi_{\alpha\beta}(ij, i'j') \mu_{\alpha}(ij) \mu_{\beta}(i'j') \\ &+ \frac{1}{3!} \sum_{i'i'', j'j''} \sum_{\alpha\beta\gamma} \Phi_{\alpha\beta\gamma}(ij, i'j', i''j'') \mu_{\alpha}(ij) \mu_{\beta}(i'j') \mu_{\gamma}(i''j'') \\ &+ \dots \end{aligned} \quad (14)$$

where α, β, \dots are the Cartesian indices. The coefficients of the series expansion, Φ_0 , Φ_{α} , $\Phi_{\alpha\beta}$, and $\Phi_{\alpha\beta\gamma}$, are the zeroth,

first, second, and third order force constants, respectively. A force and a second-order force constant $\Phi_{\alpha\beta}$ are given by

$$F_{\alpha}(ij) = -\frac{\partial\Phi}{\partial\mu_{\alpha}(ij)}, \quad (15)$$

and

$$\Phi_{\alpha\beta}(ij, i'j') = \frac{\partial^2\Phi}{\partial\mu_{\alpha}(ij)\partial\mu_{\beta}(i'j')} = -\frac{\partial F_{\beta}(i'j')}{\partial\mu_{\alpha}(ij)}. \quad (16)$$

In the phonon model with QHA, the third order force constant $\Phi_{\alpha\beta\gamma}$ as well as higher terms is ignored (harmonic approximation) and the dynamical property can be obtained from Helmholtz free energy

$$F = \frac{1}{2}\sum_{\mathbf{q}k}\hbar\omega(\mathbf{q}k) + k_{\text{B}}T\sum_{\mathbf{q}k}\ln[1 - \exp(-\hbar\omega(\mathbf{q}k)/k_{\text{B}}T)], \quad (17)$$

where the phonon frequency $\omega_{\mathbf{q}k}$ is the eigenvalue of dynamic matrix $\mathbf{D}(\mathbf{q})$,

$$D(\mathbf{q})\mathbf{e}_{\mathbf{q}k} = \omega_{\mathbf{q}k}^2\mathbf{e}_{\mathbf{q}k}, \quad (18)$$

with

$$D_{jj'}^{\alpha\beta}(\mathbf{q}) = \sum_i \frac{\Phi_{\alpha\beta}(0j, i'j')}{\sqrt{m_j m_{j'}}} e^{i\mathbf{q}[\mathbf{r}(i'j') - \mathbf{r}(0j)]}, \quad (19)$$

where m_j is mass of the atom j , \mathbf{q} the wave vector, k the band index, and $\mathbf{e}_{\mathbf{q}k}$ the polarization vector of the phonon mode, respectively.

The phonon calculations of argon and copper crystal were performed on the supercells of two face-centered cubics. Each supercell contained $7 \times 7 \times 7$ unit cells, with a total of 1372 atoms. First, we calculated the total potential energy of initial configuration using the empirical potential described above (equation (1) for argon and equation (2) for copper). The forces on each atom in the supercell were obtained by differentiating the potential energy with respect to the distance to construct the dynamic matrix \mathbf{D} in equation (19). The force constants were calculated using the Parlinski–Li–Kawazoe method [23] with a finite displacement of 0.01 Å and phonon frequencies were calculated from the force constants using the PHONOPY code [4, 24]. We obtained Helmholtz free energy F according equation (17) and the pressure can be calculated by the relation, $P = -\frac{\Delta F}{\Delta V}$, where the volume difference ΔV was made by changing the length of the box by 1%.

3. Comparisons and discussions

For the argon system of 1372 atoms with atomic volume 22.29, 26.46, 31.12 or 36.30 Å³/atom, the pressure in a temperature range from 100 to 260 K calculated by QHA (P_Q), MD (P_M) and DIA (P_D) is displayed in figure 2, showing that P_M and P_D are nearly equal to each other but significantly differ from P_Q for larger atomic volume. The relative difference (deviation) for smaller atomic volume 22.29 (or 26.46) Å³/atom, as shown by the insert of figure 2(a) (or figure 2(b)), is smaller than 2%, which approximates the accuracy of MD simulations and DIA calculations (figure 1) at temperatures above 160 K. For larger

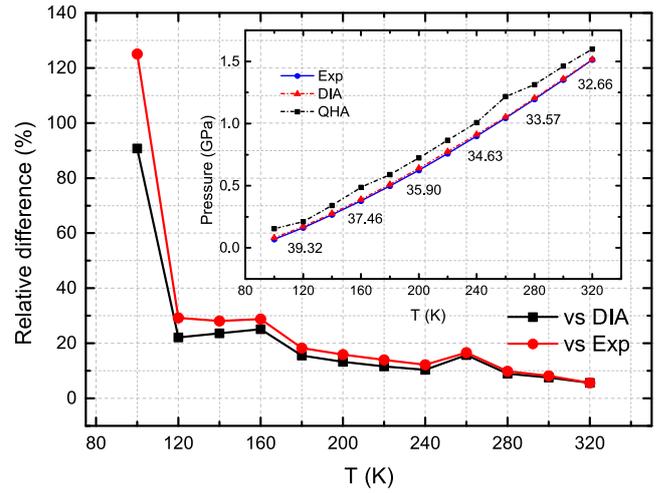


Figure 3. For the argon crystal along the melting line, the relative difference of pressure between the QHA and the experiment [14] or the DIA calculations. The inset shows their pressure values and the numbers along the curve denote the atomic volume for each temperature.

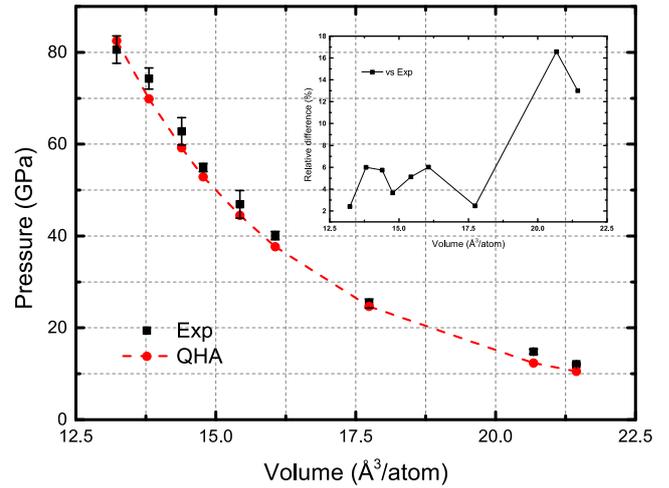


Figure 4. Volume–pressure data of compressed fcc argon at 298 K obtained by QHA (red circles) and the experiment [25] (black rectangle). The inset shows the relative difference of pressure between the QHA and experiment data. The error bars of the experiment are shown in the figure.

atomic volume (figures 2(c) and (d)), however, the deviation is significantly larger than 2% and increases up to 8% with the temperature increasing to 260 K. These results suggest a conclusion that QHA works worse and worse with the atomic volume increasing.

To confirm the above conclusion, we applied QHA to calculate the pressure of argon crystals along the melting line [14] with the atomic volume changed from 32.66 up to 40.40 Å³/atom, corresponding to the change of temperature from 320 K down to 100 K. As shown in figure 3, the calculated pressures significantly differ from the experiment values, which are in good agreement with the results of DIA. For the atomic volume of 32.66 Å³/atom, corresponding to 320 K,

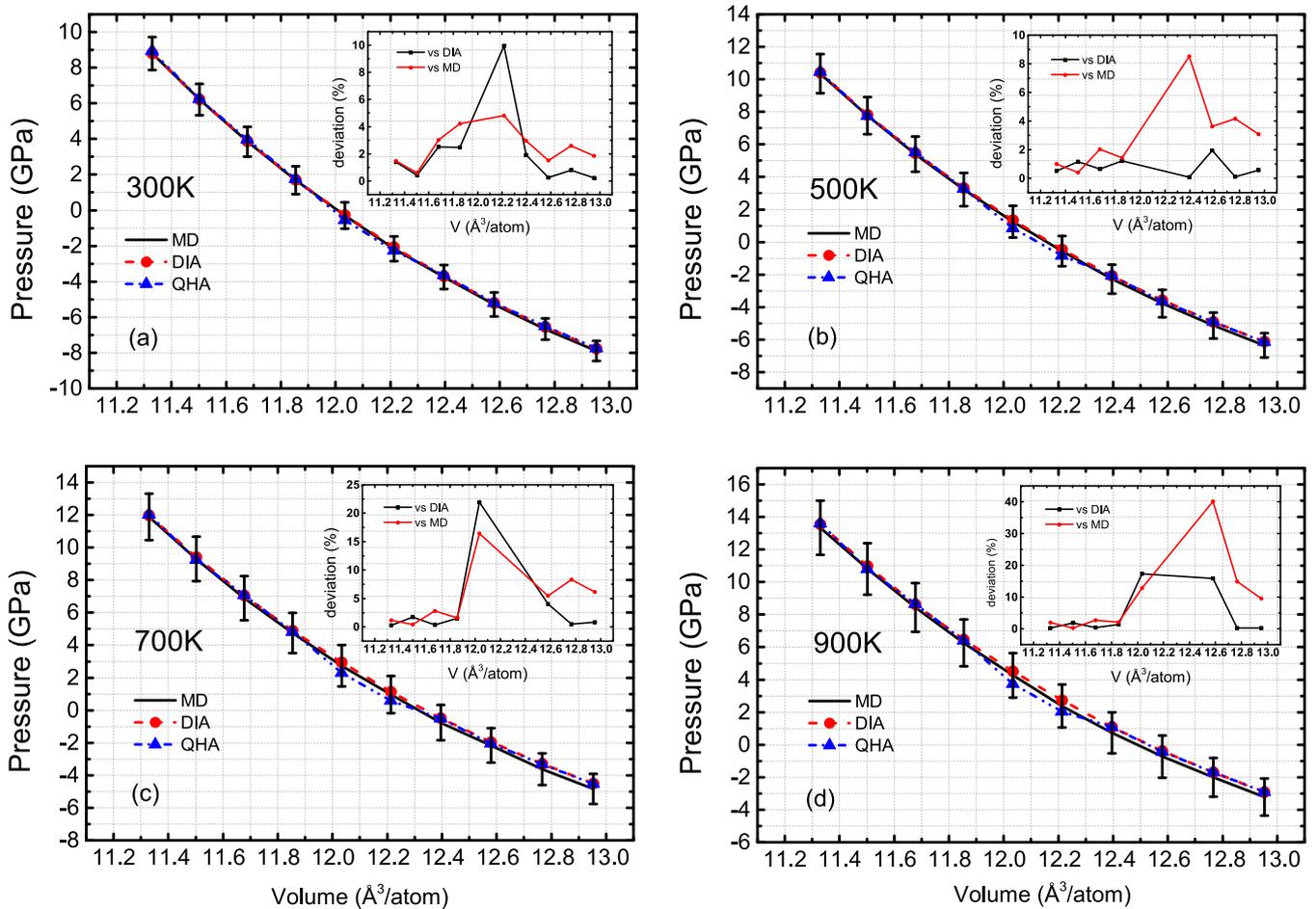


Figure 5. Pressure of 1372 copper atoms in the solid state at 300 K (a), 500 K (b), 700 K (c) and 900 K (d) with different atomic volume obtained by DIA (red circles), QHA (blue triangle) and MD simulations (black line). The insets illustrate the relative difference between QHA and MD or DIA. The error bars of MD simulations are shown in the figure.

the deviation is about 5%, and it grows gradually with the increase of the atomic volume, and reaches over 100% when the atomic volume is larger than $40.28 \text{ \AA}^3/\text{atom}$ and the temperature is lower than 120 K. For the volume–pressure data of the experiments on compressed fcc argon at 298 K [25, 26], the pressures calculated by QHA with the exponential-six potential [26] deviate from the experimental measurements by about 5% (figure 4) for the atomic volume smaller than $20 \text{ \AA}^3/\text{atom}$ (figure 4), while the deviation increases up to 15% for larger atomic volume. These result strongly supports the conclusion that the accuracy of QHA gets worse and worse with the increase of atomic volume.

In order to test the above judgment further, we considered a copper system with atomic volumes ranged from 11.3 to $13.0 \text{ \AA}^3/\text{atom}$, which are significantly smaller than the ones of the argon system. Specifically, the system consists of 1372 atoms, which were arranged in fcc sites confined within a cubic box with PBC applied, for which the same procedures of QHA, DIA and MD as for the argon systems were performed except that the interaction potential is equation (2) instead of equation (1). As shown in figure 5, the pressures from QHA are in good agreement with the results of DIA and are well

covered by the error bars of MD at 300, 500, 700 and 900 K, while the agreement for smaller atomic volume ($\leq 11.8 \text{ \AA}^3/\text{atom}$) is much better, which can be seen from the relative differences displayed in the insets of figure 5. Clearly, these results also support the above judgment. Furthermore, it is interesting to note that the atomic volume of MgO, Si, CaO and ZrO_2 crystals, for which QHA have been performed to compute the thermodynamics properties, is 18, 20, 27 and $33 \text{ \AA}^3/\text{atom}$ [5–8], which can explain why the agreement between the theory and the experiments is excellent for MgO, good for Si, but unsatisfactory for CaO and ZrO_2 even at room temperatures.

The worse performance of QHA for larger atomic volume can be explained as follows. According to equation (14), the phonon model is based on the harmonic approximation, which only validates for small displacements (μ_{α}) of the lattice atoms from the equilibrium sites. For crystals of larger atomic volume, the displacements would get larger, and the contributions to the total potential Φ from the terms higher than the quadratic term get larger, which would result in invalidation of the harmonic approximations and therefore leads to worse performance of QHA.

4. Conclusions

In summary, by comparisons with MD simulations as well as DIA calculations on pressures of argon and copper crystals, we showed that phonon model with QHA works well for crystals with smaller atomic volume but not for systems of larger atomic volume. When the atomic volume of a crystal is smaller than $20 \text{ \AA}^3/\text{atom}$, QHA should be a good approximation, and this judgment may be applicable to pre-estimate the accuracy of the phonon model for predicting the thermal dynamical properties. In addition, the DeBroglie wavelength of thermal atoms may be widely applied to judge under what condition quantum effect of thermal atoms can be ignored in classical MD simulations.

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