# Thermodynamic Properties of Solid FCC $C_{84}$ Based on an Analytic Mean Field Approach

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(Received on 4 June, 2008)

The analytic mean field potential (AMFP) approach is applied to the poly-exponential model solid. The analytic expressions for the Helmholtz free energy, internal energy and equation of state (EOS) are derived. The formalism for the case of the double-exponential (DE) model is applied to fcc $C_{84}$. One set of potential parameters are determined by fitting the experimental compression data of $C_{84}$ up to 9.24 GPa at ambient temperature (297 K). The equilibrium distance and well depth for $C_{60}$, $C_{70}$ and $C_{84}$ molecules are plotted. The thermophysical properties including the isothermals, thermal expansion, isochoric heat capacity, Helmholtz free energy and internal energy are calculated and analyzed. The theoretical results agree well with the experimental data available of $C_{84}$. Basing the results of our calculations, we may also predict the behaviors of $C_{84}$ at extreme conditions.

Keywords: Fullerenes; Analytic Mean field Potential; Equation of State; Thermodynamic Properties

## 1. INTRODUCTION

As is shown in many papers, the fullerene molecules $C_n$ are an intriguing family. $C_{84}$ is the third most abundant member of the family after $C_{60}$ and $C_{70}$ [1]. It has 24 structural isomers obeying the isolated pentagon rule; The fullerite, however, is mainly formed by only two of them, having symmetry $D_2$(IV) and $D_{2d}$(II), respectively, in a mixture of 2:1 abundance [2]. Molecules of the two isomers have almost spherical shape [2,3], and a recent experimental study has shown that solid $C_{84}$ maintains a fcc structure characterized by orientational disorder over the range 5-295 K [4]. Margiolaki *et al.* [5] have employed synchrotron X-ray powder diffraction to characterize the structural properties of pristine $C_{84}$ as a function of pressure to 9.24 GPa at ambient temperature. Their conclusion is that $C_{84}$ does not show any phase transition or irreversible transformation, being stable up to the highest pressure and its structure remaining strictly face-centered cubic. In the research of thermodynamic properties of fullerene, the pair-potential is used by many authors [6-11]. As far as $C_{84}$ is concerned, the Grifalco potential [6] has been extensively applied. Molecular dynamics simulations based on the Girifalco central two-body potential are performed by Micali *et al.* [7]. Their results for $C_{84}$ turn out to be qualitatively or semi-quantitatively accurate up to 9 GPa. Zubov *et al* [8] apply Girifalco potential to perform research on the equilibrium of $C_{76}$ and $C_{84}$ with their vapor. For the solid phase, although Zubov *et al* [9-11] improved their unsymmetrized self-consistent field (CUSF) approach and applied to $C_{60}$ and $C_{70}$, this may not to be enough at higher temperature. The reason may be that the CUSF approach cannot consider anharmonic effects soundly [12,13]. Thus, it is necessary to use other approaches that can include anharmonic effect soundly to study the thermodynamic properties of solid $C_{84}$.

It is well known that Wang et al proposed the analytic mean field potential (AMFP) method [14-17], and they applied it to many materials. Bhatt et al. [18,19] further applied the AMFP method to lead and alkali metals, and concluded that in comparison with other theoretical models the AMFP method is computationally simple, physically transparent and reliable in the study of the thermodynamic properties at high pressures and high temperatures. Recently, Sun et al. [20] proved that the AMFP method is an analytic approximation of the free volume theory (FVT). The FVT is a mean field approximation to the thermal contribution of atoms to the Helmholtz free energy of crystalline phases. Many authors [20-23] have shown that the FVT can soundly include anharmonic terms which are important at high temperatures. It is more valuable to directly use the strict FVT than the approximate AMFP, in the cases that the analytic EOS can be derived based on the strict FVT. Nevertheless, in some cases the mean field integral and the EOS for the strict FVT are fairly complicated or cannot be analytically derived. Then it is convenient to develop simple analytic EOS through the AMFP, whereas the complete FVT fails. Sun [13] has applied the AMFP method to solid $C_{60}$ by the aid of the Girifalco potential. The numerical results agree well with the MD simulations and are superior to the CUSF of Zubov et al [9,10]. This verifies that the AMFP method is a convenient approach to consider the anharmonic effect at high temperatures.

In this paper, we apply AMFP mentioned above to fcc $C_{84}$ solid. Here we also just concern the intermolecular contributions for the solid fcc $C_{84}$ as having been done by Girifalco [6,24] for $C_{60}$. Considering that the Girifalco potential has been shown too hard and gives compression curve prominently deviated from experiments at high pressure [25,26], whereas the Morse potential [27] has been shown by many authors that can well describe the thermophysical properties of most materials within wide pressure ranges, we would utilize the DE potential (an extended Morse potential) instead of the Girifalco potential.

The rest of this work is organized as follows. In Sec. II we

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derive analytic EOS based on the AMFP approach. In Sec. III the parameters of the DE potential are determined by fitting experimental data of solid $C_{84}$. And the numerical results are presented and analyzed. At last, conclusive remarks are given in Sec. IV.

## 2. ANALYTIC EQUATION OF STATE

The pair-potential $\varepsilon(r)$ of fullerene $C_{84}$ molecules can be expressed as the form of poly-exponential potential

$$\varepsilon(r/r_0) = \varepsilon_0 \cdot \sum_{j=1}^{m} C_j \exp\left[\lambda_j\left(1 - r/r_0\right)\right] \tag{1}$$

where $r$ is the radial coordinate, $r_0$ is the equilibrium distance and $\varepsilon_0$ the well depth. For the DE potential we have $m = 2$, and

$$\begin{cases} C_1 = \lambda_2/(\lambda_1 - \lambda_2) \\ C_2 = -\lambda_1/(\lambda_1 - \lambda_2) \end{cases} \tag{2}$$

The two parameters $\lambda_1$ and $\lambda_2$ describe the decay of the potential versus the radial coordinate $r$. Then the expression of potential energy $\varepsilon(r)$ involves both a repulsive term ($j = 1$) and an attractive term ($j = 2$). Our calculations show that the DE potential with $m = 2$ can describe the thermodynamic properties of solid fcc $C_{84}$ well enough, even at high-temperatures and pressures. Therefore, it is not necessary to take more terms.

In terms of the FVT, the free energy can be expressed as [6,18]

$$\frac{F}{NkT} = -\frac{3}{2}\ln(2\pi\mu kT/h^2) + \frac{u(0)}{2kT} - \ln\nu_f\ . \tag{3}$$

where $\mu$ is the mass of the $C_{84}$ molecule and $h$ Planck's constant. $u(0)$ is the potential energy of a molecule, as the lattice is static, $\nu_f$ is the free volume. The quantity $u(0)$ can be expressed as follows:

$$u(0) = \sum_{i\neq 0} z_i\varepsilon\left(\frac{R_i}{r_0}\right) = \sum_{i\neq 0} z_i\varepsilon\left(\delta_i\frac{a}{r_0}\right) = \sum_{i\neq 0} z_i\varepsilon(\delta_i y), \tag{4}$$

where $R_i = \delta_i a$ is the distance of molecules in the $i$-th shell with the centre molecule at $i = 0$. $a$ is the nearest-neighbor distance. $z_i$ and $\delta_i$ are structural constants (the values for the fcc structure have been given in [28], The quantity $y$ is the reduced volume, it is defined in equation (9). The quantity $\nu_f$ can be expressed as follows:

$$\nu_f = 4\pi\int_0^{r_m} \exp[-g(r,V)/kT]r^2 dr. \tag{5}$$

According to the AMFP method [14-17] and the cell theory, the largest displacement $r_m$ of the centre molecule can be approximately taken as the Wigner-Seitz radius $(3a^3/4\pi\gamma)^{1/3}$. Then we have $r_m = (3a^3/4\pi\gamma)^{1/3}$ in equation (5). Where $\gamma$ is a structure constant; for the fcc structure it is $\sqrt{2}$. $g(r,V)$ is the potential energy of a molecule as it roams from the centre to a distance $r$. In terms of the AMFP approach [14-17], $g(r,V)$ can be expressed by the static energy $E_c(a)$ of a molecule:

$$g(r,V) = \frac{1}{2}\left[\left(1 + \frac{r}{a}\right)E_c(a+r) + \left(1 - \frac{r}{a}\right)E_c(a-r) - 2E_c(a)\right]. \tag{6}$$

$$E_c(a) = \frac{1}{2}u(0) = \frac{1}{2}\sum_{i\neq 0} z_i\varepsilon(\delta_i y). \tag{7}$$

The volume of a fcc solid is $V = Na^3/\gamma$, ($N$ is the quantity of cell for a solid fcc $C_{84}$). For simplicity, we introduce the dimensionless reduced free volume $\bar{\nu}_f$, the reduced volume $y$, and the reduced radial coordinate $x$ as follows:

$$\nu_f = 4\pi a^3\bar{\nu}_f = 4\pi\gamma V\bar{\nu}_f/N\ . \tag{8}$$

$$y = a/r_0 = (V/V_0)^{1/3}, \quad V_0 = N(r_0)^3/\gamma\ . \tag{9}$$

$$x = r/a\ , \quad x_m = \frac{r_m}{a} = (3/4\pi\gamma)^{1/3}\ . \tag{10}$$

The reduced free volume $\bar{\nu}_f$ and its derivatives with respect to temperature and reduced volume can be expressed as

$$\bar{\nu}_f = \int_0^{x_m} \exp[-g(x,y)/kT]x^2 dx, \tag{11}$$

$$\bar{\nu}_{fa} = T\frac{\partial}{\partial T}\bar{\nu}_f = \frac{1}{kT}\int_0^{x_m} \exp[-g(x,y)/kT].g(x,y)x^2 dx, \tag{12}$$

$$\bar{\nu}_{fb} = -\frac{\partial}{\partial y}\bar{\nu}_f = \frac{1}{kT}\int_0^{x_m} \exp[-g(x,y)/kT].\frac{\partial}{\partial y}g(x,y)x^2 dx, \tag{13}$$

$$\bar{\nu}_{fc} = \frac{1}{2}\left(\frac{x_m}{y}\right)^2 \exp[-g(x_m,y)/kT] \approx 0\ . \tag{14}$$

Here $g(x,y) \equiv g(r,V)$, combining (4),(7),(9),(10), we have

$$g(x,y) \equiv g(r,V) \approx \frac{1}{4}\sum_{i\neq 0} z_i[(1+x)\varepsilon(\delta_i y + \delta_i yx) + (1-x)\varepsilon(\delta_i y - \delta_i yx) - 2\varepsilon(\delta_i y)] \tag{15}$$

$$\frac{\partial}{\partial y}g(x,y) \approx \frac{1}{4}\sum_{i\neq 0} z_i\delta_i[(1+x)^2\varepsilon'(\delta_i y+\delta_i yx)+$$

$$(1-x)^2\varepsilon'(\delta_i y-\delta_i yx)-2\varepsilon'(\delta_i y)] \tag{16}$$

$$\varepsilon'(r/r_0) = -\varepsilon_0.\sum_{j=1}^{m}\lambda_j C_j e^{\lambda_j(1-r/r_0)}. \tag{17}$$

The compressibility factor $Z$ and internal energy $U$ can be derived as

$$Z = \frac{PV}{NkT} = -\frac{y}{3}\frac{\partial}{\partial y}\frac{F}{NkT} = \frac{P_cV}{NkT}+\frac{P_fV}{NkT}, \tag{18}$$

$$\frac{P_cV}{NkT} = -\frac{y}{6kT}\frac{\partial}{\partial y}u(0), \tag{19}$$

$$\frac{\partial}{\partial y}u(0) = \sum_{i\neq 0} z_i\delta_i\varepsilon'(\delta_i y), \tag{20}$$

$$\frac{P_fV}{NkT} = 1+\frac{y}{3\bar{\nu}_f}\frac{\partial}{\partial y}\bar{\nu}_f = 1-\frac{y}{3\bar{\nu}_f}(\bar{\nu}_{fb}-\bar{\nu}_{fc}) \approx 1-\frac{y\bar{\nu}_{fb}}{3\bar{\nu}_f}, \tag{21}$$

$$\frac{U}{NkT} = -T\frac{\partial}{\partial T}\frac{F}{NkT} = \frac{3}{2}+\frac{u(0)}{2kT}+\frac{T}{\bar{\nu}_f}\frac{\partial\bar{\nu}_f}{\partial T} = \frac{3}{2}+\frac{u(0)}{2kT}+\frac{\bar{\nu}_{fa}}{\bar{\nu}_f}. \tag{22}$$

where $P_c$ is the cold pressure and $P_f$ the thermal pressure deduced from free volume.

By using the above equations, all other thermodynamic quantities can be analytically derived. The derivations are straightforward. However, the expressions for the thermal expansion coefficient $\alpha$, compressibility coefficient $\beta$ and isochoric heat capacity $C_V$ are redundant; we would calculate these quantities by using numerical differentiation instead of the analytic expressions. The compressibility factor $Z$ can be seen as a function of the variables $y$ and $T$, $Z = Z(y,T)$. In terms of the function, the formulas for the thermal expansion coefficient $\alpha$, compressibility coefficient $\beta$ and isochoric heat capacity $C_V$ can be reduced to the following form:

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{3}{y}\left(\frac{\partial y}{\partial T}\right)_P = \left[\frac{Z}{T}+\left(\frac{\partial Z}{\partial T}\right)_y\right]\left[Z-\left(\frac{y}{3}\right)\left(\frac{\partial Z}{\partial y}\right)_T\right]^{-1}, \tag{23}$$

$$\beta = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = -\frac{3}{y}\left(\frac{\partial y}{\partial P}\right)_T = \left(\frac{V_d y^3}{NkT}\right)\left[Z-\left(\frac{y}{3}\right)\left(\frac{\partial Z}{\partial y}\right)_T\right]^{-1}, \tag{24}$$

$$\frac{C_V}{Nk} = \frac{1}{Nk}\left(\frac{\partial U}{\partial T}\right)_V = \frac{U}{NkT}+T\frac{\partial}{\partial T}\left(\frac{U}{NkT}\right)_y. \tag{25}$$

In our calculations it is found that following the steps of the numerical differentiations in (23)-(25) can reach stable numerical results, $\Delta T = 0.00001\times T$ and $\Delta y = 0.00001\times y$.

## 3. NUMERICAL RESULTS AND DISCUSSION

In this section we apply the above formalism to fcc $C_{84}$. Considering the structure of the solid $C_{84}$ is fcc over the range 5-295 K [4], we thus determined one set of parameters for the DE potential by fitting the experimental compression data of $C_{84}$ up to 9.24 GPa at ambient temperature (here we have T=297 K) [5]. The experimental data and smoothed fitting curves are plotted in Fig. 1. The figure shows that the fitting precision is satisfactory. The determined values of the parameters are as follows:

$$\lambda_1 = 15.3, \quad \lambda_2 = 38.4, \quad r_0 = 1.1277nm, \quad \varepsilon_0 = 3850K \tag{26}$$

Margiolaki *et al.* [5] have used the Murnaghan EOS to analyze their experimental data, and found that the bulk modulus at atmospheric pressure and ambient temperature is 20(2) GPa, which was in good agreement with the value 19.6 GPa of solid $C_{84}$ determined by us. However, Lundin et al. [29,30] have adopted the same method to analyze their own experimental data of $C_{60}$ and $C_{70}$, they found that the bulk modules at ambient pressure for $C_{60}$ and $C_{70}$ are 6.8 GPa and 7.6 GPa, respectively. This means the bulk modulus on compar-

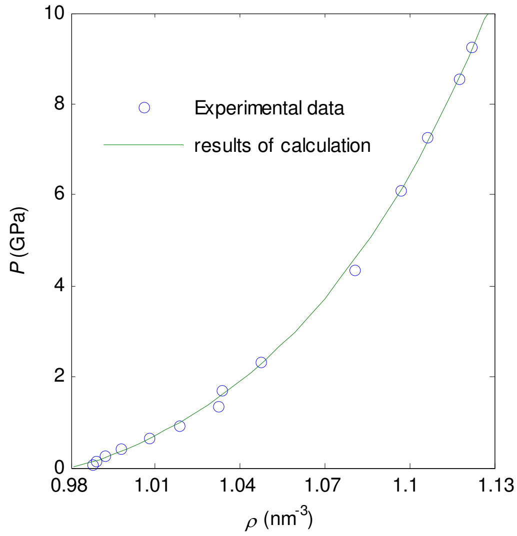


FIG. 1: Pressure as function of density for fcc $C_{84}$ solid at 297 K by using the parameters of (26). Comparison of the results of our calculation (lines) with the experimental data (circles) [5].

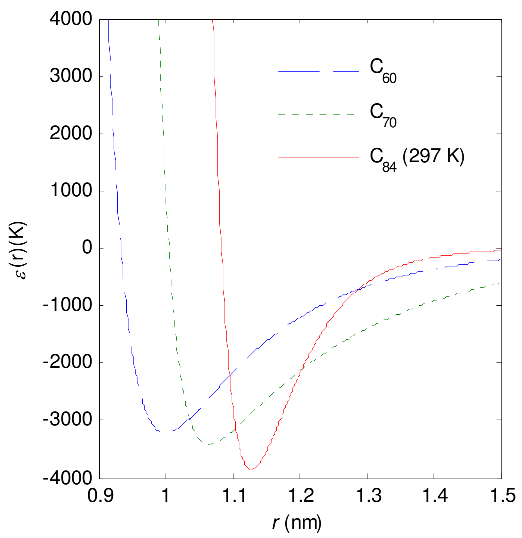


FIG. 2: Comparison of the DE potential of the $C_{60}$, $C_{70}$ molecules with the $C_{84}$ molecules' at 297 K.

ison with $C_{60}$ and $C_{70}$ solid shows that $C_{84}$ solid is hardly compressible. The potentials for $C_{60}$, $C_{70}$ and $C_{84}$ molecules are plotted in Fig. 2. We notice that the well depth of $C_{60}$, $C_{70}$, $C_{84}$ molecules is 3219 K, 3410 K and 3850 K, respectively. It shows that the intermolecular interaction between the $C_{84}$ molecules is stronger than that between the $C_{60}$ molecules and $C_{70}$ molecules, respectively. The conclusions are in good agreement with the results of experiments. The difference of tendency among the potentials for $C_{60}$, $C_{70}$ and $C_{84}$ molecules is fairly small at high-pressure, but at low pressure the difference become prominent, the attractive of the DE potential for $C_{84}$ is harder than those for $C_{60}$ and $C_{70}$.

The thermodynamic properties calculated at zero-pressure and different temperatures by using the parameters of (26) are listed In Table 1. The spinodal point $T_s$ is the temperature satisfying the condition $B_T(T_s) = 0$. The system is unstable for temperatures above $T_s$. From the table we know that $T_s$ is 2807 K for the parameters of (26). At the same time, we noticed that the $T_s$ of $C_{60}$ and $C_{70}$ is 2440 K and 2635 K, respectively [31,32]. Thus we can obtain the following sequence, $T_s$ ($C_{84}$) $>$ $T_s$ ($C_{70}$) $>$ $T_s$($C_{60}$). This means that the fullerene solids can keep stable at higher temperature for fullerene with heavier molecules. The table 1 shows that the thermal expansion coefficient and lattice constant are the increasing functions of temperature, whereas the bulk modulus and the isochoric heat capacity are decreasing function of temperature. And the thermal expansion coefficient becomes divergent and the bulk modulus tends zero near the spinodal temperature.

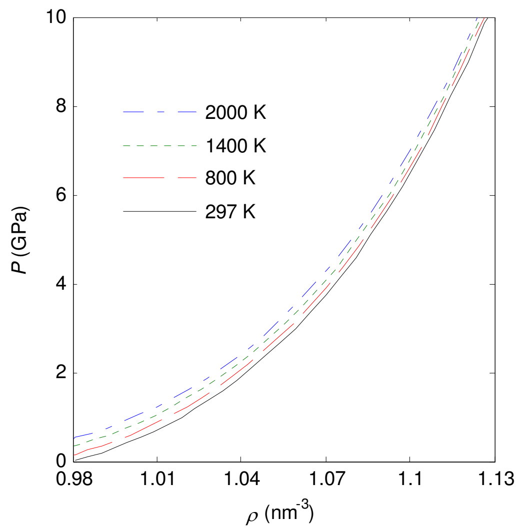


FIG. 3: Isothermal curves at 297 K, 800 K, 1400 K, 2000 K calculated by using the parameters of (26).

In Figs. 3-8, we plotted the results of thermodynamic properties of fcc $C_{84}$ solid calculated by using the DE potential. The isothermal curves at 297 K, 800 K, 1400 K, 2000 K calculated by using the parameters of (26) are plotted in Fig. 3. The results suggest that the density of $C_{84}$ increases with pressure and decreases with temperature. The variations of bulk modulus $B_T$ versus pressure $P$ at the same temperatures are plotted in Fig. 4. The $B_T$ is a linear increasing function of pressure, but the slope is fairly large and the increase is fast. This means the DE model solid for fcc $C_{84}$ is difficult to be compressed.

Fig. 5 and Fig. 6 give the variation of thermal expansion coefficient and isochoric heat capacity $C_V$ versus pressure $P$ at 297 K. Fig. 5 shows that $\alpha$ is a decreasing function of pressure $P$, at low pressure the variation is fast, but at high pressure, the variation slows down and shows some saturation effect. Fig. 6 shows that $C_V$ is an increasing function of pressure $P$, and the variation is fast at low pressure and is slow at high pressure. The calculated free energy $F$ and internal energy $U$ as function of the density $\rho$ for $C_{84}$ at four temperatures (297 K, 800 K,

TABLE I: Thermophysical properties of the fcc phase of $C_{84}$ at zero-pressure calculated by using the parameters determined from the experimental data [5] at 297 K: the lattice constants $a$ in nm, linear thermal expansion coefficient $\alpha$ in $10^{-5}K^{-1}$, the bulk modulus $B_T$ in GPa, the heat capacity $C_V$ in $kJ.mol^{-1}.K^{-1}$.

| $T$ | 200 | 400 | 600 | 800 | 1000 | 1200 | 1400 | 1600 | 1800 | 2000 | 2200 | 2400 | 2600 | 2807 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $a$ | 1.5966 | 1.5986 | 1.6007 | 1.6029 | 1.6053 | 1.6079 | 1.6107 | 1.6139 | 1.6174 | 1.6214 | 1.6262 | 1.6322 | 1.6405 | 1.6634 |
| $\alpha$ | 0.6011 | 0.6359 | 0.6760 | 0.7226 | 0.7777 | 0.8437 | 0.9247 | 1.0269 | 1.1606 | 1.3449 | 1.6199 | 2.0894 | 3.1616 | 86.488 |
| $B_T$ | 19.074 | 17.613 | 16.177 | 14.765 | 13.374 | 12.0 | 10.641 | 9.2936 | 7.9526 | 6.6111 | 5.2572 | 3.8675 | 2.3805 | 0.0071 |
| $C_V$ | 24.616 | 24.304 | 23.986 | 23.662 | 23.331 | 22.989 | 22.633 | 22.259 | 21.859 | 21.424 | 20.937 | 20.368 | 19.639 | 17.930 |

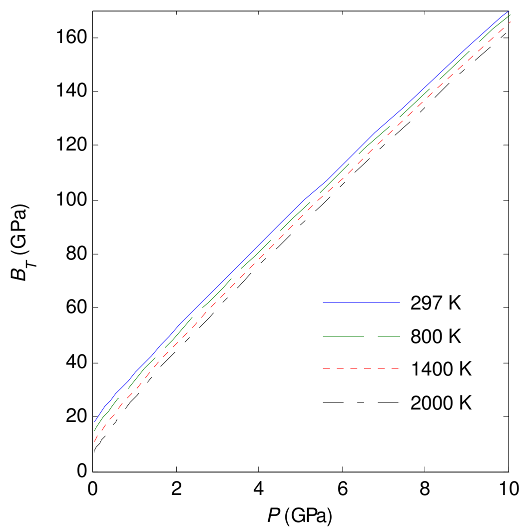


FIG. 4: Variations of bulk modulus $B_T$ versus pressure $P$ at the same temperatures in Fig. 3. The bulk modulus is in GPa.

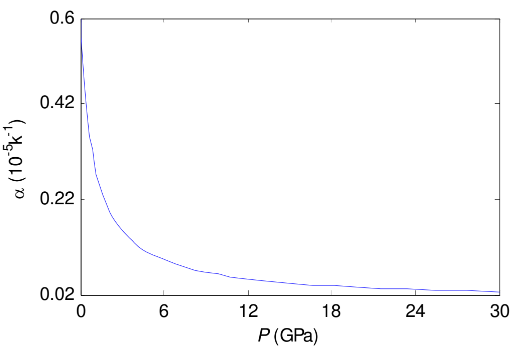


FIG. 5: (297 K) Variation of thermal expansion coefficient $\alpha$ versus pressure $P$ calculated in this work. The linear thermal expansion coefficient in $10^{-5}K^{-1}$.

1400 K, 2000 K) are plotted in Fig. 7 and Fig. 8, respectively. The two figures show that both the free energy $F$ and internal energy $U$ of $C_{84}$ are increasing function of the density $\rho$ and the two physical quantities have the same variation tendency as the density $\rho$ increase at four different temperatures. The variation at high density condition is faster than that at low density condition. On the other hand, the two figures also show that $F$ and $U$ are increasing functions of temperature under the condition of the fixed density.

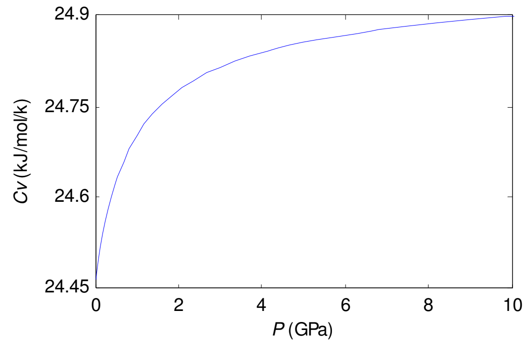


FIG. 6: (297 K) Variation of isochoric heat capacity $C_V$ versus pressure $P$ calculated in this work. The heat capacity is in $kJ.mol^{-1}.K^{-1}$.

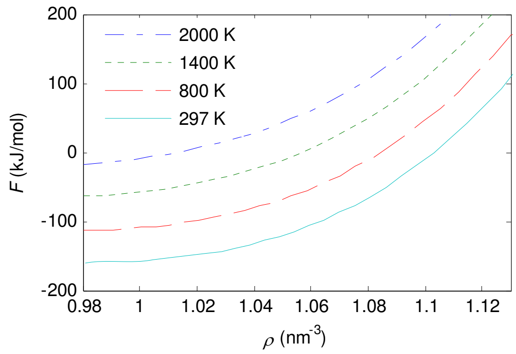


FIG. 7: Variation of free energy $F$ versus density $\rho$ at 297 K, 800 K, 1400 K, 2000 K calculated by using the parameters of (26). Here the contribution of ideal gas to free energy is neglected.

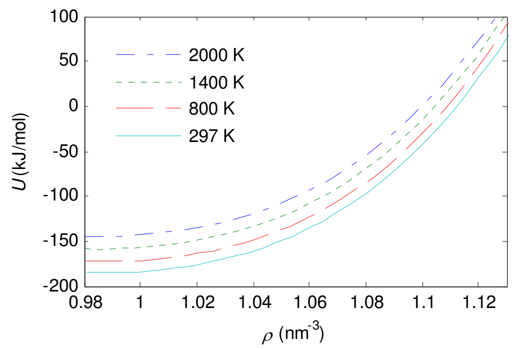


FIG. 8: The same as for Fig. 7, but for internal energy $U$.

## 4. CONCLUSION

In summary, the analytic expressions on equation of state and internal energy for the poly-exponential solid have been derived based on the AMFP method. The formalism developed is applied to the fcc $C_{84}$ solid. One set of potential parameters are determined through fitting the experimental compression data of $C_{84}$ up to 9.24 GPa at ambient temperature. The calculation results agree well with the available experimental data and the other authors' results calculated by using different methods. These results presented in this paper verify that the AMFP method is a useful approach to consider the anharmonic effects at high temperature. In the present paper, numerous reasonable predictions and the change trend of the properties for $C_{84}$ at extreme conditions have been given.

**Acknowledgements**

This work was supported by the Support Programs for Academic Excellence of Sichuan Province of China under Grant No. 06ZQ026-010, that of the Education Ministry of China under Grant No. NCET-05-0799, and that of UESTC under Grant No. 23601008.

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