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Self-consistent statistical thermodynamics of an anharmonic one-dimensional crystal surface under pressure

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ABSTRACT

In this work, we use the unsymmetrized self-consistent field theory and the Gibbs's method of excess functions to calculate surface thermodynamic properties of an anharmonic one-dimensional crystal surface under pressure. We find an overall decrease in the anharmonicity while increasing the pressure. Using some specific interatomic potential functions, we are able to corroborate the analytical results.

1. Introduction

In statistical physics, the equilibrium properties of crystalline solids are more appropriately described by the isothermal–isobaric ensemble since temperature and pressure are the external parameters for most experimental situations in which a solid can be placed [1]. Furthermore, when we are interested in the lattice dynamics of a real solid, anharmonicity must be considered. This approach becomes important because it is these anharmonic effects that will describe several thermodynamic phenomena. It is these effects that generate coupling between different modes of oscillation, that is anharmonicity is the mechanism related to the exchange of energy between mechanical and thermal vibrations [2].

The effect of pressure on the vibrational and thermodynamic properties of a solid, taking into account the anharmonicity, is not yet fully understood. Correspondingly, few studies have been carried out, such as self-consistent phonon theory [3–6], density functional perturbation theory [7], Raman spectra [8], and path integral Monte Carlo [9]. Concerning the surface properties of a crystal, the situation is even worse although one can find some attempts such as the quantum quasi-harmonic approximation [10,11]. In its turn, regarding the recent advances in experimental realizations of low dimensional systems [12–14], it remains current the problem of the account of pressure in the theoretical approaches as is the case of the unsymmetrized self-consistent field (USF) theory [15–17]. This method has proved to be efficient in the study of anharmonic crystals, including the theory of surfaces and defects [18–23]. This statistical theory allows us to calculate at finite temperature structural, dynamical, and thermodynamic properties with anharmonic effects up to the higher orders without the need of employing perturbative methods.

Naturally, one has to consider the finite size of a crystal to take into account the effect of external pressure, which is akin to the force applied to the surface. Any mechanical contact between two solid surfaces or a fluid and a solid might originate this force.

In the present work, we investigate the effect of pressure on the surface thermodynamics properties of a phenomenological model [24] of a solid, regarding the action of a force field through an effective potential V. The extent of this force

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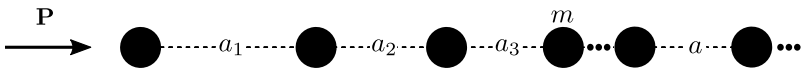

Fig. 1. The semi-infinite chain of atoms with mass m under an external force P; a_i are the average interatomic distances and a the interatomic distance in the infinite chain.

field can be determined by parameters that define some external constraint, such as the kinetic gas pressure, its mass or concentration.

2. The unsymmetrized self-consistent field approximation

The Liouville equation for the distribution function of a macroscopic system can be reduced to BBGKY hierarchy of equations for the reduced probability functions [25]. To truncate them different approximations are used. For instance, the two-particle function is usually approximated by the product of one-particle functions [25],

$$W_{ij}(x_i, p_i; x_j, p_j) = W_i(x_i, p_i)W_j(x_j, p_j). \tag{1}$$

It assumes that the particles are not correlated in their motion while their mutual interactions are expressed by a mean-field potential created by all the others [25]. This approximation is suitable for systems in which each particle moves in a field created simultaneously by a great number of other particles; in crystals this condition is met because of the sufficient number of nearest neighbors and also because the amplitudes of atomic oscillations are small.

In general, the distribution function is assumed to be symmetric with respect to transposition of identical particles [26]. However, in the statistical theory of crystals the symmetry condition when used together with the product approximation leads to several inconsistencies [27] such as an equal probability to find each atom in any cell of the crystal and a great probability of several atoms located in the same cell [15]. In a crystal each atom vibrates around its corresponding lattice site and the probability of transition to other lattice sites is small. Because of that the distribution function of the crystal must be unsymmetrical with respect to the coordinates and momenta of identical particles.

Unsymmetrical distribution functions with respect to transposition of identical particles can be used in classical statistical mechanics [15,28]. Each particle moves by its own trajectory and transposition of identical particles must lead to new microstates of the system and then their joint probability in general does not have to be symmetric. The unsymmetrical description of a system of spatially separated particles is possible in quantum mechanics too [29].

In this approximation, each atom of the crystal is described by its own one-particle probability density that decreases rapidly with the distance from the correspondent lattice site. Let us consider a semi-infinite linear chain with nearest-neighbor interactions as the simplest model of a crystal with a surface. In Fig. 1 we illustrate this model. The Hamiltonian of this model is

$$H = \sum_{i=1}^{N}\left[\frac{p_i^2}{2m} + V(x_i)\right] + \sum_{i=1}^{N-1}\Phi\left(x_i - x_{i+1}\right), \tag{2}$$

where V is an external field and Φ is the pairwise interatomic potential. In the equilibrium the first system of equations of the unsymmetrical BBGKY hierarchy for our model is

$$\frac{p_i}{m}\frac{\partial W_i}{\partial x_i} - \sum_{j=1}^{N}\left(1-\delta_{ij}\right)\int \frac{\partial \Phi}{\partial x_i}\frac{\partial W_{ij}}{\partial p_i}\,dx_j dp_j - \frac{\partial V}{\partial x_i}\frac{\partial W_i}{\partial p_i} = 0. \tag{3}$$

Approximating the two-particle function by the product of one-particle functions (1), the hierarchy of system of equations is truncated in the first system Eqs. (3) given a closed system of N nonlinear integro-differential equations for the one-particle distribution functions,

$$\frac{p_i}{m}\frac{\partial W_i}{\partial x_i} - \left[\sum_{j=1}^{N}\left(1-\delta_{ij}\right)\int \frac{\partial \Phi}{\partial x_i}W_j\,dx_j dp_j + \frac{\partial V}{\partial x_i}\right]\frac{\partial W_i}{\partial p_i} = 0. \tag{4}$$

The coordinates separate and the dependence of the momenta has the usual Maxwellian form while for the spatial parts $w_i(x_i)$ a system of N nonlinear integral equations is obtained

$$\ln\left[\Lambda_i w_i(x_i)\right] + \frac{1}{\theta}\left[\sum_{j=1}^{N}(1-\delta_{ij})\int \Phi(x_i - x_j)w_j(x_j)\,dx_j + V(x_i)\right] = 0, \tag{5}$$

where as usually $\theta = k_B T$, k_B being the Boltzmann's constant, T the absolute temperature and the constants Λ_i are determined by the normalization conditions

$$\int w_i(x_i)\,dx_i = 1. \tag{6}$$

The Eqs. (5) and (6) are the basic equations of the USF approximation for crystals with pairwise central forces.

3. The solution of the basic equations

It is usual here the change of variables $x_i = a(i-1) + q_i$, where the new spatial variables q_i are the displacements of the particles from their equilibrium positions. Here, a is the distance between particles in the undistorted system, i.e. in the infinite linear chain $a = a_P + \Delta a(\theta)$, where $\Delta a(\theta)$ is the thermal expansion. The static analysis of the semi-infinite chain with a force P applied to the tip atom gives an implicit expression for a_P

$$\Phi^{\mathrm{I}}(a_P) = -P. \tag{7}$$

The force P comes from the effective external potential V whose action is limited only to the tip atom

$$V(x_i) = -Px_i\delta_{i1}. \tag{8}$$

The basic Eqs. (5) and (6) can be written in the form,

$$w_i(q_i) = \frac{\exp\left[-\dfrac{u_i(q_i)}{\theta}\right]}{\displaystyle\int \exp\left[-\frac{u_i(q_i)}{\theta}\right] dq_i}, \tag{9}$$

where $u_i(q_i)$ is the ith atom self-consistent potential

$$\begin{aligned} u_i(q_i) = \sum_{j=1}^{N}(1-\delta_{ij})\Bigg[\int \Phi(a(i-j)+q_i-q_j)w_j(q_j)\,dq_j \\ - \frac{1}{2}\int \Phi(a(i-j)+q_i-q_j)w_i(q_i)w_j(q_j)\,dq_i dq_j\Bigg] \\ + V(a(i-1)+q_i), \qquad i = 1, 2, \ldots, N. \end{aligned} \tag{10}$$

It is different from that one that appears in square brackets in (5) which is the one usually applied in the statistical and quantum mechanical methods, by the addition of a constant term dependent on the thermodynamic parameters that changes the origin of counting the potentials [16]. With this change one eliminates the double counting of the energy of interatomic interactions. Moreover, although the self-consistent potential do depend on temperature the mean value of this derivative turns out to be equal to zero, the mean exact and self-consistent potential energies end up being equal, and the thermodynamic functions take then the usual Gibbsian form. A variational approach to obtain (10) is given in [19].

The usual technique to solve the USF basic Eqs. (9) and (10) is to expand the pairwise potential in power series of the relative displacements of the atoms from their equilibrium positions [18,19], thereby

$$u_i = u_{i_0} + \sum_{\ell=1}^{\infty}\frac{1}{\ell!}F_\ell^i q_i^\ell - Pq_i\delta_{i1}, \tag{11}$$

where the constants u_{i_0} are defined as

$$u_{i_0} = \frac{1}{2}\left(F_0^i - \sum_{\ell=1}^{\infty}\frac{1}{\ell!}F_\ell^i\overline{q_i^\ell}\right) - P(i-1)a\delta_{i1}, \tag{12}$$

and the expansion coefficients F_ℓ^i are given by

$$\begin{aligned} F_\ell^1 &= \sum_{k=0}^{\infty}\frac{1}{k!}(-1)^\ell\Phi^{(\ell+k)}(a)\overline{q_2^k}, \\ F_\ell^i &= \sum_{k=0}^{\infty}\frac{1}{k!}\left[(-1)^k\Phi^{(\ell+k)}(a)\overline{q_{i-1}^k} + (-1)^\ell\Phi^{(\ell+k)}(a)\overline{q_{i+1}^k}\right], \end{aligned} \tag{13}$$

for $i = 2, \ldots, N$. Thus, the Eqs. (9), (11), (12), (13) and

$$\overline{q_i^k} = \int q_i^k w_i(q_i)\,dq_i \tag{14}$$

are reduced to a system of transcendental equations for the moments of the one-particle distribution functions (14).

In the case of strong anharmonicity, these transcendental equations can be solved only numerically. Here though, we shall consider the approximation of weak anharmonicity which is valid for not too high temperatures. The anharmonic terms in the power series are considered as small compared to the harmonic ones. Thus the series (11) is separated in three parts, a constant one, a second one with the harmonic terms, and a third one with the anharmonic terms including those of the first power. Then the exponential functions in (9) are factored and the factor with the anharmonic terms is

expanded in power series. As a result, the transcendental equations are linearized and a system of algebraic equations is obtained for the moments of the one-particle distribution functions (14). The solution of these algebraic equations gives the moments as expansions in power series of temperature [18]. Usually, when considering anharmonic terms up to the fourth order implies taking in to account terms up to the second order in temperature.

To calculate the thermal expansion, the thermal equation of state for an infinite linear chain is used [18]. The interatomic potential and their derivatives are expanded in power series of the thermal expansion taking into account terms up to the second order of temperature. For the thermal expansion we obtain

$$\Delta a(\theta) = -\frac{g_P\theta}{2f_P^2}\left[1+\frac{\theta}{f_P^2}\left(\frac{3}{4}\frac{g_P^2}{f_P}-h_P+\frac{f_Pk_P}{4g_P}\right)\right]. \tag{15}$$

Here and in what follows we use for the values of the interatomic potential and its derivatives taken at the equilibrium position a_P the notations,

$$\epsilon_P = \Phi(a_P); \quad e_P = \Phi^{\mathrm{I}}(a_P); \quad f_P = \Phi^{\mathrm{II}}(a_P); \quad g_P = \Phi^{\mathrm{III}}(a_P); \quad h_P = \Phi^{\mathrm{IV}}(a_P); \quad k_P = \Phi^{\mathrm{V}}(a_P). \tag{16}$$

In this approximation, we use the condition that moving along the atomic chain the odd moments vanish

$$\lim_{i\to\infty}\overline{q_i^{2n+1}} = 0, \tag{17}$$

which means that surface effects such as the relaxation of the chain and the softening of the atomic vibrations fade away. In the approximation of weak anharmonicity with the boundary condition (17) and the expansion of the interatomic potential and its derivatives in the equilibrium position a_P, the solution of the system of algebraic equations for the moments is obtained for our model. The first order moments, that express the relaxation of the chain are obtained as

$$\begin{aligned}
\overline{q_1} &= \frac{g_P\theta}{4f_P^2}\left[1+\frac{\theta}{2f_P^2}\left(\frac{23}{4}\frac{g_P^2}{f_P}-\frac{19}{3}h_P+\frac{5}{4}\frac{f_Pk_P}{g_P}\right)\right],\\
\overline{q_2} &= \frac{g_P\theta^2}{32f_P^4}\left(\frac{g_P^2}{f_P}-h_P\right),\\
\overline{q_i} &= \mathcal{O}(\theta^3), \quad i\geq 3.
\end{aligned} \tag{18}$$

The second order moments describe the effective amplitudes of vibration. For them the following expressions are obtained

$$\begin{aligned}
\overline{q_1^2} &= \frac{\theta}{f_P}\left[1+\frac{\theta}{4f_P^2}\left(\frac{21}{4}\frac{g_P^2}{f_P}-3h_P\right)\right],\\
\overline{q_2^2} &= \frac{\theta}{2f_P}\left[1+\frac{5}{8}\frac{\theta}{f_P^2}\left(\frac{g_P^2}{f_P}-h_P\right)\right],\\
\overline{q_i^2} &= \frac{\theta}{2f_P}\left[1+\frac{\theta}{2f_P^2}\left(\frac{g_P^2}{f_P}-h_P\right)\right], \quad i\geq 3.
\end{aligned} \tag{19}$$

Finally, the third and fourth order moments that describe the asymmetry and other less intuitive characteristics of the distribution functions are obtained as

$$\overline{q_1^3} = \frac{7}{4}\frac{g_P\theta^2}{f_P^3}, \qquad \overline{q_i^3} = \mathcal{O}(\theta^3), \quad i\geq 2 \tag{20}$$

$$\overline{q_1^4} = \frac{3\theta^2}{f_P^2}, \qquad \overline{q_i^4} = \frac{3}{4}\frac{\theta^2}{f_P^2}, \quad i\geq 2. \tag{21}$$

It turns out that the expressions obtained here for the thermal expansion and for the moments of the distribution functions have the same form as for the case of the absence of the external force [18]. The difference is that in this case the interatomic potential and its derivatives are taken not at the equilibrium point a_0, ($\Phi^{\mathrm{I}}(a_0) = 0$) but at the point a_P obtained by (7).

In the USF method, the choice of the interatomic potential Φ is arbitrary. Here, we choose the attractive–repulsive (m, n) two-body potential function

$$\Phi(x) = \epsilon\frac{m}{(m-n)}\left(\frac{m}{n}\right)^{n/(m-n)}\left[\left(\frac{\sigma}{x}\right)^m-\left(\frac{\sigma}{x}\right)^n\right], \tag{22}$$

where ϵ is the depth of the potential and σ is a bond length. Two particular cases are $(12, 6)$ and $(m, 0)$ for Lennard-Jones (LJ) and soft-repulsion (SR), respectively [30]. The values of the parameters ϵ and σ ($\sigma = a_0/2^{1/6}$) are taken correspondent to the case of solid Xenon for some numerical estimates of our analytical results. For the SR potential, the exponent m indicates the rigidity of the repulsive interaction. In this work, we show numerical results for the case $m = 12$.

Using the solutions of the algebraic equations for the moments we can now construct the one-particle distribution functions. In Fig. 2 we show the behavior of these functions in the space (p, x) along the chain for different pressures for

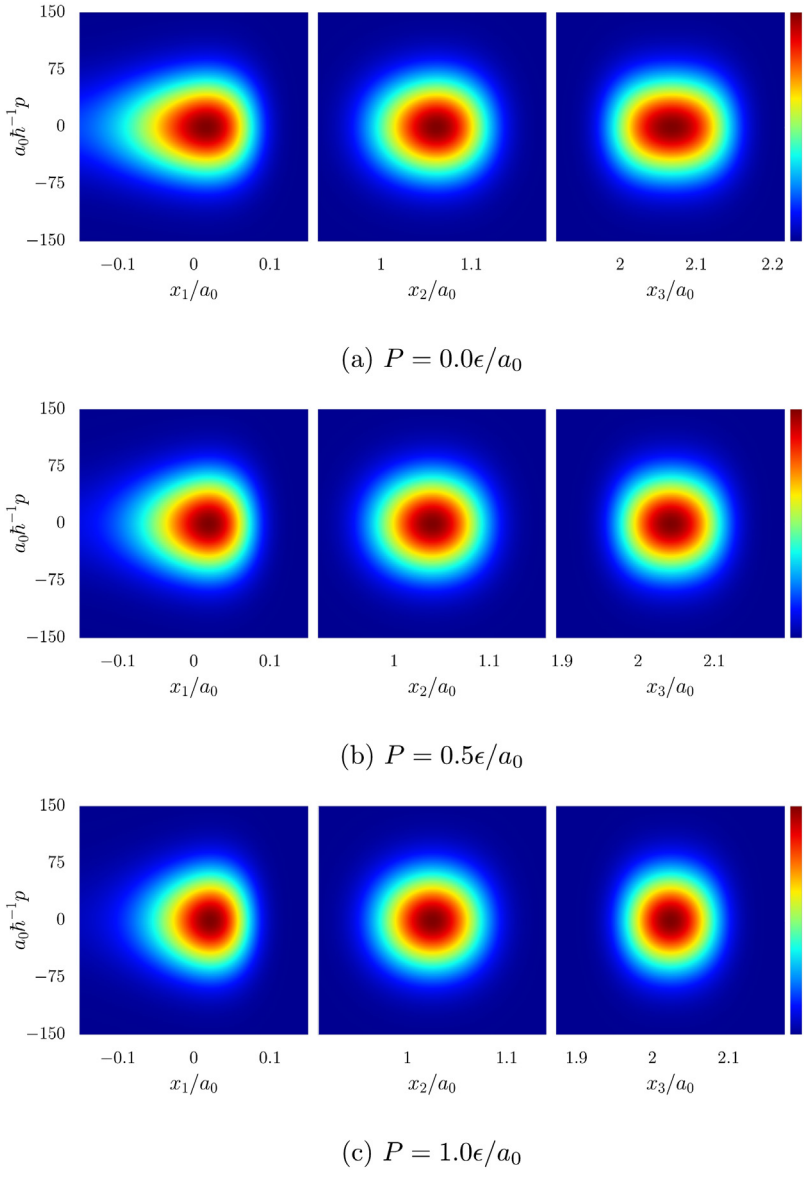

Fig. 2. Classical phase space of the first three particles of the semi-infinite chain for different values of pressure.

the case of the two-body Lennard-Jones potential at the temperature $\theta = 2.0 \times 10^{-1}\epsilon$. The asymmetry observed at the tip ("surface") of the chain is a surface effect. Inside the chain this asymmetry disappears. In the present approximation, this occurs starting from the third atom of the chain from which the existence of a surface no longer can change the symmetry of the chain. By applying an external force, the whole distribution changes. To the edge of the chain the increase of pressure leads to a weakening of the surface effects. For the other atoms, the reach of the distribution becomes smaller due to the external pressure yielding a decrease in the effective amplitudes of vibration. Besides, the anharmonic effects increase sharply with temperature.

4. Surface specific heat

In the approximation (1) the Helmholtz free energy is determined by the usual Gibbsian formula. Therefore it is possible to calculate quantum corrections to these quantities [31]. The possibility of these corrections comes from the application of the formal Wigner–Kirkwood expansions in the USF theory [17,19]. In this quasi-classical approximation the Helmholtz

free energy of our model contains a first quantum correction [32] which is of second order in $\hbar^2$,

$$F = -\theta \ln \left\{ \left(\frac{m\theta}{2\pi\hbar^2} \right)^{N/2} \int \exp\left[-\frac{1}{\theta} \sum_{i=1}^{N} u_i(q_i) \right] dq_i \right\} + \frac{\hbar^2}{24m\theta} \sum_{i=1}^{N} \overline{\frac{\partial^2 u_i(q_i)}{\partial q_i^2}}. \tag{23}$$

In order to obtain the equations of state in the isothermal–isobaric ensemble first one has to build the Gibbs thermodynamic potential defined as [33]

$$G(\theta, P) = F(\theta, L(\theta, P)) + PL(\theta, P). \tag{24}$$

Here, L is the length of the chain and can be given as

$$L(\theta, P) = (N-1)(a_P + \Delta a) + \frac{1}{2}(a_P + \Delta a). \tag{25}$$

The expression PL is roughly equal to PV where V here is the volume of the crystal. Here we use first quantum correction [32] for the thermal expansion (15). Adding the Eqs. (23) and (25), integrating and substituting the expressions obtained for the thermal expansion (15) and the self-consistent potentials u_i in the previous section, we obtain

$$G = \frac{1}{2}(\epsilon_P + Pa_P) + \frac{\hbar^2}{24m\theta}\left(f_P - \frac{Pg_P}{f_P} \right) + \frac{\theta}{2} \ln\left(\frac{\hbar^2 f_P}{m\theta^2} \right) + \frac{\theta^2}{16 f_P^2}\left(3h_P - \frac{29}{6}\frac{g_P^2}{f_P} \right) + (N-1)\frac{G^{\mathrm{id}}}{N}, \tag{26}$$

where $\frac{G^{\mathrm{id}}}{N}$ is the Gibbs thermodynamic potential per atom in the ideal (infinite) chain

$$\frac{G^{\mathrm{id}}}{N} = \epsilon_P + Pa_P + \frac{\hbar^2}{12m\theta}\left(f_P - \frac{Pg_P}{f_P} \right) + \frac{\theta}{2} \ln\left(\frac{2\hbar^2 f_P}{m\theta^2} \right) + \frac{\theta^2}{8 f_P^2}\left(h_P - \frac{g_P^2}{f_P} \right). \tag{27}$$

In the USF the classical internal energy is determined by the formula

$$\overline{E} = \frac{1}{2}N\theta + \sum_{i=1}^{N} \overline{V(x_i)} + \sum_{i=1}^{N-1} \overline{\Phi\,(x_i - x_{i+1})}, \tag{28}$$

thus, one can readily verify the validity of the Gibbs–Helmholtz equation

$$G - \theta\left(\frac{\partial G}{\partial \theta} \right)_P - P\left(\frac{\partial G}{\partial P} \right)_\theta = \overline{E}. \tag{29}$$

This means that the results are thermodynamically compatible. Notice that when differentiating with respect to pressure P one has to use the expression (7) and also the relations resulting from (7) by successive differentiation's

$$\frac{da_P}{dP} = -\frac{1}{f_P}; \quad \frac{d\epsilon_P}{dP} = \frac{P}{f_P}; \quad \frac{df_P}{dP} = -\frac{g_P}{f_P}; \quad \frac{dg_P}{dP} = -\frac{h_P}{f_P}; \quad \frac{dh_P}{dP} = -\frac{k_P}{f_P}. \tag{30}$$

In order to determine the "surface" thermodynamic potentials, the terms proportional to N must be subtracted. This yields the "excess" free and internal energies which are characteristic of the Gibbs's approach to the thermodynamic description of surface [34]. The "volume" in this treatment is a region localized below the surface (the volume of the surface phase is assumed to be zero, i.e. the surface is treated as a geometrical layer; in the one-dimensional case it is a point). The layer is located in such a way that the "excess density" is equal to zero, i.e. the equimolecular surface. It is clear from this procedure that in the calculation of G the volume and the surface are assumed to have a meaning which is strictly equivalent to the Gibbs's method. In our case, the reference system is the ordered infinite linear chain that is the quantity proportional to the number of particles N.

The specific heat at constant pressure is given by

$$c_P = -k_B\theta\left(\frac{\partial^2 G}{\partial \theta^2} \right)_P, \tag{31}$$

and so the excess part relates to the surface specific heat,

$$\frac{c_P^{\mathrm{sur}}}{k_B} = \frac{\hbar^2}{12m\theta^2}\left(f_P - \frac{Pg_P}{f_P} \right) + \frac{\theta}{8 f_P^2}\left(\frac{17}{6}\frac{g_P^2}{f_P} - h_P \right) \tag{32}$$

and for the ideal system one has

$$\frac{c_P^{\mathrm{id}}}{Nk_B} = 1 + \frac{\hbar^2}{6m\theta^2}\left(\frac{Pg_P}{f_P} - f_P \right) + \frac{\theta}{4 f_P^2}\left(\frac{g_P^2}{f_P} - h_P \right). \tag{33}$$

For the case of Lennard-Jones potential, the ideal specific heat increases in the high-temperature regime, since the anharmonicity becomes more and more essential. This result is in agreement with other theoretical methods and experimental results [6,7,9]. While for the soft-repulsion potential the ideal specific heat decreases in the same range

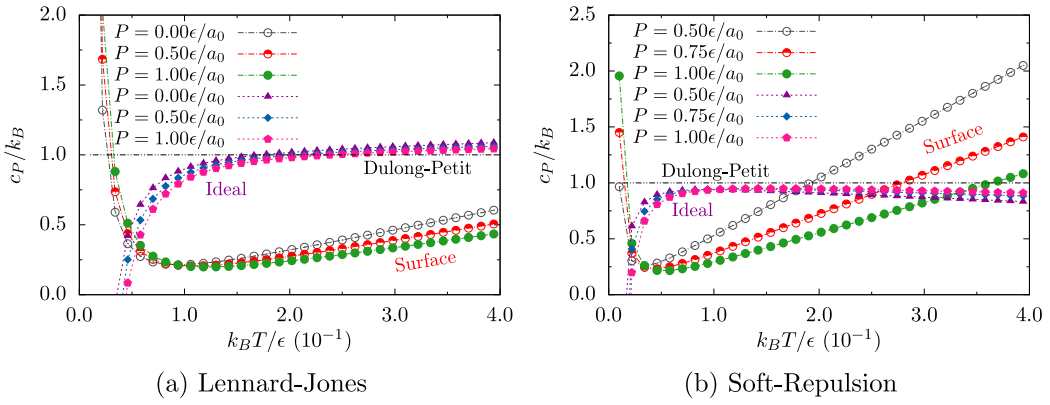

Fig. 3. The specific heat (surface and ideal) versus the temperature for both LJ and SR interactions.

of temperature. This behavior is similar to the specific heat at constant volume (Fig. 3). Thus the attractive part in the interatomic potential is relevant for the determination of the behavior of the thermodynamic properties. It is like the interatomic interaction could considerably change the thermal behavior of the matter. The increasing of the pressure at the surface causes both the behaviors to tend to the Dulong–Petit law limit.

When observed the effect of surface in both models of interaction potentials, (LJ and SR), the same dependence on temperature is seen except that in the absence of the attractive term the surface atom has a greater degree of freedom and that leading a noticeable increase of the surface specific heat for the case of the soft-repulsion model. Besides, the surface vibrational modes grow up with the rise of temperature since the anharmonic effects dominate in this regime. For low temperatures, the surface modes grow up indefinitely in the quasi-classical approximation though it is known that in the quantum theory of solids there is a maximum value in the surface specific heat in the quasi-harmonic approximation [10,11]. Since the external field reduces the effective amplitudes of vibration one can speculate that the external field will decrease the modes at the surface too and consequently reduce the peak in the regime of low temperatures. By taking greater values for the index of rigidity m there will be more increase of c_P for the surface, whereas for the ideal case there will be a decrease. The results obtained here using the quasi-classical anharmonic theory are in agreement with those given by the quantum quasi-harmonic theory [10,11].

5. Final remarks

In conclusion, we have shown here that the unsymmetrized self-consistent field approximation is an efficient tool in the analysis of a macroscopic model of solid with a surface under the action of an external field. Besides, in this method there is no need to resort to perturbation techniques in order to take into account higher-order anharmonic terms. We have solved the algebraic equations in the weak anharmonic approximation up to the second order in temperature for the moments of the classical one-particle distribution functions and therefrom we have calculated the partition function and thereafter the specific heat in the second order of temperature. The first quantum correction has been calculated. To calculate these properties for the surface, which in the one-dimensional case is the edge of the semi-infinite chain, we have employed the description of excessive functions developed by Gibbs. We conclude that the external field applied to the surface leads to an overall decreasing of the anharmonic effects. Having analyzed the problem of the ordered semi-infinite chain, we now could continue by studying the problem of a chain with a topological disorder. However, this problem is much more complex due to the absence of symmetry although it is still possible to be treated analytically using the unsymmetrized self-consistent field theory. This theory can be generalized to the higher dimensional case.

CRediT authorship contribution statement

Rodrigo S. Amorim: Investigation, Writing - original draft, Visualization. **Cláudio J. DaSilva:** Writing - review & editing, Term, Conceptualization. **J.N. Teixeira Rabelo:** Methodology, Investigation, Writing - original draft, Writing - review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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