Structural phase-field crystal model for Lennard–Jones pair interaction potential

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Abstract

A modification of the structural phase-field crystal model for a Lennard–Jones (LJ) pair interaction potential is presented. Formation of 1D and 2D structures for the LJ-potential was studied numerically. The equilibrium lattice parameters for the obtained structures were found consistent to the correspondent LJ-distance parameters. The lattice parameter of 2D triangle’s structure matches the periodical in 1D, which is consistent to the theory of freezing from the isotropic liquids. Numerically obtained phase diagram of two-dimensional structures qualitatively reproduces classical PFC diagram and coincides with the melting region of high-temperature part of LJ diagram.

Keywords: phase-field crystal, structural phase-field crystal, pair interaction potentials, pair correlations, Lennard–Jones potential

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

1. Introduction

The phase-field crystal model (PFC) was formulated [1–5] to describe continuous transitions from the homogeneous to the various periodic states (similarly to the Landau–Brazovskii transitions [6–8]) and between them over diffusion times. The model is based on the description of a Helmholtz free energy, which is a functional of the atomic density field which is periodic in the solid phase and homogeneous in the liquid (disordered) state. Recent advances in PFC-modeling of the different aspects of crystallization allow one to describe many scenarios such as dynamics of freezing of colloids and polymers, epitaxial growth, ordering on nano-scales [9–11] and rapid crystallization [12]. The PFC model is able to provide interface
energies, reproduces pattern selection, multiphase solidification under non-equilibrium conditions, heteroepitaxy and multi-grain growth in presence of hydrodynamical flows [13–19]. As a simplification of a classical density functional theory (cDFT) of freezing [20, 21] the PFC model utilizes several approximations [2, 22] leading to the overall behavior similar to the systems with hard-spheres potential. The PFC-model predictions were validated using the molecular dynamics simulations [15, 23, 24]. But at the same time, rough PFC approximations lead to a bit of criticism concerning about accuracy of calculating of surface energies on long times and problems with quantitative description of elastic properties and set of emerging structures [25, 26].

The form of the classical PFC free energy is close to the Swift–Hohenberg equation [1, 27] and in general allows one to describe phase transitions of the first and second order [28]. To robust the structural transitions later, the artificial multipeaked correlation kernels were introduced to the PFC models [4, 29]. Such kernels based on so-called structural PFC (XPFC) were generalized for a multi-component metallic systems [16, 30–32] and stable 3D structures such as diamond [25, 33]. Several cases of the formation of two-dimensional structures were also examined for the three-point correlation functions [34, 35]. Those improvements of XPFC model mostly regard to the modification of the position and size of first and second peaks of correlation function in a reciprocal space ($k$-space). It was shown that stabilization of graphene-like structure requires not only a repulsive term but a rotationally invariant correlation function of higher approximation [36]; such extension is also capable to stabilize kagome lattice [37] for the case of three-mode PFC. The multiscale PFC-like model were proposed by [38] where the excessive energy term was expanded in the reciprocal space in two components: short ‘condensation’ term and spherically symmetrical long-range interaction term. Obtained results clearly state that the repulsive term is sufficient for the ‘structural’ crystallization in the presence of a middle-range attraction written in the form of row of derivatives. In [38] a quasi-continuous approximation of the phase-field were proposed for the case of discrete values (1 or 0) of the atomic density in each lattice node (about 8 nodes per lattice period). Expansion of the direct correlation functions with quadratic terms in the reciprocal space was carried out by [39] for the cDFT. Such approach in fact is very close to the idea of eight-order [40] and twelve-order [41, 42] fitting in PFC. Although, a derivation of PFC as a consequent approximation of dynamical density functional theory with the gradient expansion leads to the possible instability above a certain value of an average density [26]. A comprehensive stability analysis of the emerging PFC structures was proposed in [43]. A promising approach consisted in approximation of the pair-correlation interactions by the rational functions is discussed in [44].

In present work we propose a modification of the structural phase-field crystal (XPFC) model with the Lennard–Jones (LJ) pair interaction potential. A study of the structure formation and crystallization from the undercooled liquid (homogeneous) phase was carried out. In particular, the equilibrium lattice parameters, sequence of the emerged structures and their phase diagram were studied.

2. Classical density functional theory of freezing and phase-field crystal model

The classical PFC equation obtained from approximation of the cDFT is suitable for the description of the crystallization of liquids to the simple crystalline structures [1, 9, 21, 40, 45]. The derivation of this model is based on the approximation of cDFT free energy of single-particle’s probability density field $\rho(r, t)$ which is a function of spatial coordinate $r$ and time $t$. 
Let one consider the static isothermal approximation of cDFT free energy containing ideal and excess free energies neglecting any external potential [1, 20, 46, 47]:

$$F[\rho(r)] = F_{id}[\rho(r)] + F_{ex}[\rho(r)].$$ (1)

The ideal contribution $F_{id}$ corresponds to the free energy functional of Boltzmann gas [1, 9, 46], here any particles interactions were neglected:

$$F_{id}[\rho(r)] = k_B T \int d^3 r \rho(r) (\ln(\lambda^3 \rho(r)) - 1),$$ (2)

where $k_B$ is the Boltzmann constant, $T$ is temperature, $\lambda$ is the thermal de Broglie wavelength. Let one substitute normalized (by the reference density $\rho_0$) averaged atomic density field $n(r) = \rho(r)/\rho_0 - 1$ to equation (2):

$$F_{id}([\rho(r)]) = k_B T \rho_0 \int d^3 r [(1 + n(r)) \ln(1 + n(r)) - n(r)].$$ (3)

The second term $F_{ex}[\rho(r)]$ of the equation (1) corresponds to the excess energy of the particles exchange interactions. To determine it explicitly, it is necessary to make a number of approximations [21, 46, 47]. The exact expression of $F_{ex}[\rho(r)]$ as a generating functional can be formally obtained with the expansion around the small density change $\tilde{\rho}(r) = \rho(r) - \rho_0$. Its expansion over time-independent (slowly varying) density field $\tilde{\rho}$ would be [20, 21, 48, 49]:

$$F_{ex}[\rho(r)] = F_{ex}[\rho_0] + \int d^3 r \tilde{\rho}(r) \frac{\delta F_{ex}[\rho(r)]}{\delta \rho(r)}$$

$$+ \frac{1}{2} \int d^3 r d^3 r' \tilde{\rho}(r) \tilde{\rho}(r') \frac{\delta^2 F_{ex}[\rho(r)]}{\delta \rho(r) \delta \rho(r')},$$

$$+ \frac{1}{6} \int d^3 r d^3 r' d^3 r'' \tilde{\rho}(r) \tilde{\rho}(r') \tilde{\rho}(r'') \frac{\delta^3 F_{ex}[\rho(r)]}{\delta \rho(r) \delta \rho(r') \delta \rho(r'')} + \cdots$$ (4)

These functional derivatives of the excess energy are related to the $n$-body direct correlation functions $C^{\alpha\beta\gamma\cdots}(r_1, r_2 \ldots r_n)$:

$$\frac{\delta^n F_{ex}[\rho(r)]}{\delta \rho(r_1) \delta \rho(r_2) \cdots \delta \rho(r_n)} = -k_B T C^{\alpha\beta\gamma\cdots}(r_1, r_2 \ldots r_n).$$ (5)

Substituting the excess energy with direct correlation functions equation (4) to (1), truncating it up to 2nd term of equation (5) and considering the normalized atomic density $n(r)$ one can get a dimensionless free energy:

$$F(n) = \frac{\mathcal{F}}{k_B T \rho_0} = \int d^3 r [(1 + n(r)) \ln(1 + n(r)) - n(r)]$$

$$- \frac{1}{2} \int d^3 r \int d^3 r' C ||r - r'|| n(r'),$$ (6)

where $C ||r - r'||$ is the pair correlation function. Here the free energy is scaled by the energy of a reference state: $\mathcal{F} = F[\rho(r)] - F[\rho_0]$. The pair correlation function could be approximated in a reciprocal space (space of $k$-vectors) in a manner proposed by Ramakrishnan and Yusoff (RY) [20, 21] leading to the ‘standard’ PFC-model [2, 3].
3. Structural PFC model for arbitrary interaction potentials

3.1. Structural PFC model

This structural PFC (XPFC) utilizes a reduced expansion of the pair correlation function \( C(r) \) in a row of exponents. The later development of XPFC consists in the approximation of a three-point correlation function as a sum of pair-correlation functions which includes repulsive and anisotropic terms [34, 35]. This artificial correlation functions allow one to reproduce stable hexagonal lattices, which also can be modeled with the three-mode isotropic PFC model [37].

The XPFC free energy in the dimensionless case could be derived from equation (6) using the Taylor expansion of \( F_{id}(n) \) term around the reference density \( n(r) = 0 \) with the expansion coefficients \( a \) and \( v \) [2, 3]:

\[
F_{id}(n) = (1 + n) \ln(1 + n) - n \approx \frac{1}{2}n^2 - \frac{a}{3}n^3 + \frac{v}{4}n^4. \tag{7}
\]

Moreover such free energy term allows one to describe first- and second-order phase transitions [28, 40]. The full free energy of the XPFC model is now read as:

\[
F(n) = \int dr \left[ \frac{1 - \varepsilon}{2} n^2 - \frac{a}{3}n^3 + \frac{v}{4}n^4 \right] - \frac{1}{2} \int dr \int dr' C(|r - r'|n(r'), \tag{8}
\]

where \( \varepsilon \) is the dimensionless driving force \( \varepsilon = (\Delta B_0 - \Delta B_0^*)/\Delta B_0^* \) with the critical driving force value \( \Delta B_0^* \) corresponding to the melting temperature \( T_m \) [36, 41].

3.2. Correlation function for arbitrary interaction potentials

The RY approximation of the non-local part of the free energy describing freezing transitions equation (8) inputs the pair correlation function of fluid. One can obtain this pair-correlation function in the analytical form from the liquid integral equation theory [49]. Practically, for a case on the non-negligible interactions one can assume a deviation from an ideal gas in a form of virial equation of state which was previously introduced in [9, 50]. The second-order virial coefficient, which has a physical meaning of direct pair correlation function, can be analytically approximated for an arbitrary pair interaction potential \( U(r - r') \) leading to the virial expression [49–51]:

\[
C(r - r') = \exp \left( \frac{-U(r - r')}{k_BT} \right) - 1 \tag{9}
\]

The correspondent distribution function becomes asymptotically exact to the Boltzmann factor of the pair potential in the low density limit [49]. In present paper we propose the LJ potential [52] for benchmarking of the XPFC with the arbitrary interacting potential:

\[
U(r - r') = \varepsilon_U \left( \frac{r_m}{r - r'} \right)^{12} - 2 \left( \frac{r_m}{r - r'} \right)^6, \tag{10}
\]

where \( \varepsilon_U \) is the depth of the potential well, \( r_m \) is the LJ-distance parameter. This potential includes the long-range attraction as well as repulsive component what is required for the crystallization process. The classical LJ potential allows solidification to different crystalline structures [53, 54] from a LJ-liquid. The possible phase diagram is broader than simple structural hard-sphere solidification, which lays underline the classical-PFC approximation [20]. The similar idea for description of binary LJ-mixtures using the cDFT is utilized with the different approximations of short- and long-range interactions [55]. It is important to point out,
that LJ-liquid naturally freezes into FCC solid in three dimensions [56], which differs from a hard-sphere-like PFC-models resulting BCC-crystal [57]. In figure 1(a) the direct space pair correlation function obtained for LJ-potential equation (10) with virial expression equation (9) is presented, parameters are $\epsilon_U = 1$, $r_m = 1$, $k_B T = 1$. Now we transfer to the reciprocal space to compare one-mode PFC $C(k) = C_0 + C_2 k^2 - C_4 k^4 + \cdots$ (where $C_n$ are the gradient expansion coefficients) and LJ with the virial approximation, see figure 1(b). As one can see the PFC model reproduces only the first peak of pair correlation function $C(k)$. In more complex case $C(k)$ can be approximated with the rational function fit [44] to carefully reproduce the higher modes.

3.3. Dynamical equations

The PFC and XPFC conserved dynamics for atomic density $n$ is described with equations [1, 3]:

$$\frac{\partial n}{\partial t} = \nabla^2 \mu(n), \quad \mu(n) = \frac{\delta F(n)}{\delta n},$$

(11)

where $\mu(n)$ is a chemical potential defined by the functional derivative (Gateaux) of the free energy equation (6) as a sum of two terms:

$$\mu = \frac{\delta F_{\text{id}}(n)}{\delta n} + \frac{\delta F_{\text{ex}}(n)}{\delta n}.$$  

(12)

To find the dynamical equation for the XPFC model we consider the convolution integral of excess part of the XPFC free energy equation (8). This functional term $F_{\text{ex}}(n)$ enters the functional derivative (Gateaux) for the dynamical PFC equation. Let one introduce the test function $\theta(r)$ and a small $\epsilon \to 0$ so the Gateaux variation for this convolution will be:

$$\frac{d}{d\epsilon} \frac{F_{\text{ex}}(n + \epsilon \theta)}{\epsilon = 0} = \frac{d}{d\epsilon} \int dr \int dr' C(r - r') n(r') (n(r) + \epsilon \theta(r')) \bigg|_{\epsilon = 0}$$

(13)

$$= \frac{d}{d\epsilon} \int dr \int dr' C(r - r') n(r') \epsilon \theta(r') + n(r') \epsilon \theta(r) + \epsilon \theta(r) \epsilon \theta(r')) \bigg|_{\epsilon = 0}.$$  

(14)

Here the term $\epsilon \theta(r) \epsilon \theta(r')$ is neglected by the order of magnitude as a small parameter. Resulted functional derivative is

$$\frac{\delta F_{\text{ex}}(n)}{\delta n} = -\frac{1}{2} \left( \int dr n(r) C(r - r') + \int dr' C(r - r') n(r') \right).$$  

(15)
which allows one to describe the dynamics in the structural-PFC model for the arbitrary pair correlation function. Considering the isotropic correlation function this convolution becomes:

\[ \frac{\delta F_{\text{ex}}(n)}{\delta n} = - \int dr' C||r - r'|| n(r'), \quad (16) \]

where \( C||r - r'|| \) is the arbitrary pair correlation function in direct space. This function can be obtained in the reciprocal space using the convolution theorem [34, 35]. The fitting of this function is possible with rational function fitting procedure [44]. Also for the calculations in direct space one can use the similar approximation with help of expansion of this convolution integral into two complex parts. In case of analytical form of \( C(r) \) in direct space one can introduce the direct convolution integration to the numerical procedure presented in the next section. Resulted XPFC chemical potential after substitution of the functional derivative equations (16) to (12) will be:

\[ \mu(n) = (1 - \varepsilon)n(r) + an(r)^2 + vn(r)^3 - \int dr' C(r - r')n(r'). \quad (17) \]

3.4. Numerical implementation

One can split equation (11) with (17) reducing the order of spatial derivatives:

\[
\begin{cases}
\frac{\partial n}{\partial t} = \nabla^2 \mu, \\
\mu = (1 - \varepsilon)n + an^2 + vn^3 - \int dr' C(\xi)n(r'),
\end{cases}
\quad (18)
\]

where \( \xi = |r - r'| \). To deal with the solution divergence at \( \xi = 0 \) we use LJ-potential equation (10) in the form:

\[ U(\xi) = \varepsilon_U \left( \left( \frac{r_m}{\xi + K} \right)^{12} - 2 \left( \frac{r_m}{\xi + K} \right)^{6} \right), \quad (19) \]

where \( K = 0.01 \) is a small shift constant. The system of equation (18) has been solved numerically in one- and two-dimensions in direct space using a direct solver PARDISO for the finite element method with the linear-C1 Lagrange elements utilizing the COMSOL Multiphysics Software [58] on two-processor AMD Epyc 7302-based computer with 64 cores and 1024 Gb of RAM. To perform convolution kernel integration we use a COMSOL realization of moving-boundary integrals \( \text{intop()} \) with \( \xi = x - \text{dest}(x) \) (example is given in one-dimensional case), where operator \( \text{dest()} \) corresponds to the moving boundary. To reach the convergence the \( \text{nojac()} \) operator for the convolution integral has been used; this operator omits the nonlinear Jacobian contribution from the current step and use the approximation from the previous one. Thus the size of adaptive time step has been limited by \( \delta t = 10^{-3} \). The initial density field was set as \( n_0 \), crystallization was initiated by introducing the single disturbance at the edge of the domain. The two-dimensional computational domain consists of \( L_x \times L_y = 10 \times 12 \) dimensionless units with the triangle grid of maximum size \( \ell = 0.3 \); the size of the one-dimensional domain is \( L_x = 50, \ell = 0.1 \). The periodic boundary conditions were introduced.
Figure 2. Free energy profiles for the periodical solution equation (20) as a function of wave number \( q \) for the one-dimensional XPFC equation (8) with LJ-potential obtained for various parameters of LJ-distance \( r_m \), driving force \( \varepsilon \), density \( n_0 \).

4. Solutions of one-dimensional XPFC equation

The search for the equilibrium lattice parameter \( \lambda \) in the PFC models is of considerable interest.

We performed a numerical minimization of the free energy functional integrated in the limits of a single unit cell \( 0 \leq x \leq 2\pi/q \), where \( q \) is a wave number. The simple periodical solution could be written in the form

\[
n = n_0 + \eta \cos(qx),
\]

where \( n_0 \) is the initial density, \( \eta \) is the PFC amplitude. After substituting of equation (20) to the XPFC free energy equation (8) with analytical correlation function equation (9) for LJ-potential equation (10) one can plot a free-energy profiles, see figure 2. Minimization of \( \eta \) was performed numerically. We calculated the preferable wave numbers \( q \) for different LJ-potential’s parameters and found an inverse dependence of \( q \) on \( r_m \) parameter. One can see a presence of distinct minima correspondent to the preferable \( q \) for every profile. We found that \( q = 3.7 \) for \( r_m = 1.4 \), \( q = 2.7 \) for \( r_m = 2 \), and \( q = 1.72 \) for \( r_m = 3 \). This also coincides to the value of minimum of LJ-potential which equals to \( r = r_m^{1/6} \) [52]. The change of the driving force (undercooling) \( \varepsilon \) in the region of stable existence of periodic phase leads only to the change of PFC amplitudes \( \eta \) and quantity of \( F \) but not to the change of the position of minimum, e.g. equilibrium wave number \( q \). As a generalized driving force contribution, initial density \( n_0 \) also affects only on severity and relative well depth. Reduction of the density \( n_0 \) is followed by the decreased stability of the periodic phase. When the system approaches to the melting line the minimum disappears.

The numerical solutions of XPFC equation (18) for LJ-potential are shown in figure 3. The relatively large interface width is very close to the one shown for the XPFC model with exponential kernel with \( \alpha = 2 \), reference [29]. We found the equilibrium lattice parameter \( \lambda = 2.3 \), which totally coincides with the correspondent wave number \( q = 2.7 = 2\pi/\lambda \) obtained by the minimization of \( F \) figure 2. The artifacts of the numerical integration procedure is quite noticeable near the edges. Here we see the main problem of the presented implementation of
the direct convolution integration. Since the integration is being held for the whole domain, the integration radius is not limited, nevertheless, the integration on boundaries does not give the exact values in the primary peak correlation radius. Thus the additional development of the numerical implementation is needed. In such case, the reciprocal Fourier spectral method \cite{44} looks promising but it also raises the problem of the consideration of the arbitrary boundary conditions and implementation for asymmetrical domains. Besides of that, the real space implementation can improve calculation speed with adaptive mesh refinement; however one cannot expect the unconditional convergence of the numerical scheme in the reciprocal space for the non-rational polynoms including the functions in the form of LJ-potential. In present work we focused on the implementation of XPFC model with the arbitrary $C(r)$ kernel with direct finite element scheme in the context of our previous works \cite{59, 60}. In addition, our proposed method differs from Helmholtz equations method from \cite{44} by direct introduction of the integration of $C(r)$ over the whole domain.

5. Solutions of two-dimensional XPFC equation

Results of the numerical simulations of 2D XPFC-model equation (18) with LJ-potential are presented in figure 4. For the LJ-distance parameter value $r_m = 1.4$ we did not get any stable triangle structures. Instead we found a spinodally decomposed homogeneous (liquid) phase with confluent stripe-like phase boundary, figure 4(a), and coexistence of striped and liquid phases figure 4(b). This can be caused by the difficulties in stabilization of the periodic phase at low-range $r_m$, see the correspondent shallow well in figure 2. The other reason is caused by the basic property of the PFC models which suppress the high-frequency harmonics leading
Figure 4. Snapshots of the numerical solutions of 2D XPFC with LJ-potential obtained for different parameters are given at fixed time $t = 150$. Column 1, $r_m = 1.4$: (a) $\varepsilon = 0.1$, $n_0 = -0.1$; (b) $\varepsilon = 0.5$, $n_0 = -0.5$. Column 2, $r_m = 2$: (c) $\varepsilon = 0.1$, $n_0 = -0.5$; (d) $\varepsilon = 0.2$, $n_0 = -0.2$. Column 3, $r_m = 3$: (e) $\varepsilon = 0.3$, $n_0 = -0.5$; (f) $\varepsilon = 0.4$, $n_0 = -0.05$.

to the destruction of subtle high-frequency phases [59, 61]. Obtained triangle structure is consistent with the one obtained in the PFC models [62], see figure 4(c), where the case $r_m = 2$ is considered. The LJ-distance parameter $r_m = 2$ was also utilized for the construction of phase diagram, see figure 5. The sample of coexistence region of triangles and striped phase for $r_m = 2$ is shown in figure 4(d). The sample snapshots for $r_m = 3$ is presented in figures 4(e) and (f). Here the mixed triangles-striped and striped-inverted triangles structures are shown respectively. The boundary artifacts caused by the integration are especially noticeable here. The lattice parameters obtained in this simulations can be compared to the equilibrium ones from the free energy minimization: for $r_m = 2$ in 2D we got for triangles $\lambda_\Delta = 2.32$ and for stripes $\lambda_\Diamond = 2.04$; for $r_m = 3$ triangles $\lambda_\Delta = 3.57$, stripes $\lambda_\Diamond = 3.02$. One can notice a difference between $\lambda$ for triangle and striped structures, meanwhile $\lambda_\Delta$ matches the related $\lambda$ for the simple 1D periodic lattice, see figure 2, and correspondent equilibrium $\lambda$ obtained from $r_m$.

Triangle crystal appears as a preferable structure during crystallization in the theory of freezing from the isotropic liquids; in two dimensional case one can consider triangle symmetry as a simplest crystalline symmetry [57]. This symmetry in 2D is analogue to the simplest possible regular periodical structure in 1D. For 3D case such simplest and most preferable structure is BCC [57]. The lattice matching between $\lambda_\Delta$ and $\lambda$ in 1D is related to this fact as soon as the liquid in XPFC model could be considered as a constant isotropic phase.

Here we present the numerically obtained phase diagram of two-dimensional structures for XPFC model with LJ-potential. Such stable structures qualitatively coincide with the classical PFC (see diagram in [62]). We obtained three regions of existence of triangles, stripes and liquid (homogeneous) phases. Results of performed numerical experiments are depicted with the correspondent symbols in figure 5. The analytical curve has been obtained using the thermodynamical method [62] with the numerical minimization of triangles and homogeneous free energies and Maxwell area rule. The several boundary marks could correspond to the coexistence regions of the adjacent phases such as presented in figure 4(d). Obtained phase diagram qualitatively corresponds to the high-temperature region of 2D LJ diagram obtained with molecular dynamics [63]. Although, the striped phase is not observed in LJ diagram. The
Figure 5. Numerically obtained phase diagram ‘driving force, $\varepsilon$—initial density, $n_0$’ for the XPFC model with LJ-potential for $r_m = 2$. The types of relaxed structures are designated with the correspondent symbols: ◦—liquid (homogeneous) phase, △—triangle lattice, ◆—striped phase. The analytically obtained melting curve depicted as a solid line.

6. Conclusions

In present work we introduce the modification of the XPFC model for LJ pair interaction potential. The pair interactions is approximated using the second order term of the virial expansion and thus with the analytical form of the pair correlation function. We studied the presented XPFC model with simple LJ potential in one- and two-dimensional cases. The numerical implementation is also presented and discussed. The crystallization from the undercooled homogeneous liquid to the solid crystalline phase was carried out. In one-dimensional case the equilibrium lattice parameters were calculated and compared to the LJ-distance parameters and numerical solutions. The two-dimensional numerical simulations was performed and resulted liquid, triangles, striped phases and their mixtures. With the obtained numerical data the lattice parameters for each structure was calculated. The lattice parameter’s values of the two-dimensional triangle and one-dimensional periodical structure are exactly matched to each other and to the correspondent LJ-distance parameters. The set of obtained numerically structures and the phase diagram by itself qualitatively coincide to the classical PFC model, the form of the melting region is consistent with the high-temperature region of two-dimensional LJ diagram.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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