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Behavior of condensed inert gases at the phase line of melting near transition between attraction and repulsion of atoms

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We consider the properties of condensed inert gases as an atomic system with pairing interaction between nearest atoms on the phase line of melting, when attraction and repulsion between atoms change one to other. Zero point corresponds to pressure about of 10 GPa. Experimental method of diamond anvil allows us to obtain pressures up to 100 GPa. According to experimental data, switching of interaction is non-singular point. Therefore, the pressure on the phase line of melting increases monotonic with temperature. We suggest the interaction potential between two identical atoms of an inert gas. One of the border corresponds to repulsion with the interaction potential of 0.3 eV. The other border corresponds to the bottom of the potential well. Parameters of the potential are determined from the experimental data for the thermal conductivity coefficient at high temperatures. In the switching region, jumps of atomic density and of the internal energy are relatively small. Therefore, the jump of the internal energy due to variation of structure of atomic system becomes significant. We found the criteria of observed behavior of condensed inert gases at the phase transition in the region, which corresponds to the positive jump of atomic density and of the internal energy both in the case of attraction, as in the case of repulsion.

Keywords: melting phase line, exchange interaction of inert gas atoms, diamond anvil method.

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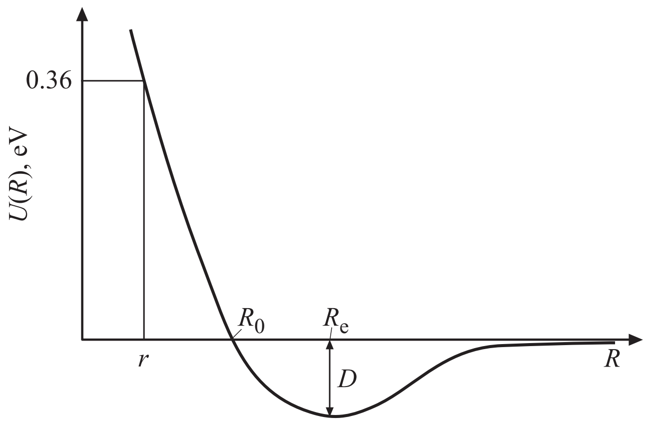
1. Introduction

Analysis of condensed inert gases as the simplest dense system of interacting atoms allows understanding the principal problems of fluids and solid bodies. This analysis is simplified in virtue of the pairwise nature of interaction between the atoms and domination of interaction between the closest neighbors [1]. The principal role in such analysis is played by experimental data. It is the experiment that proves reliably the existence of fluid and solid aggregate states. The method of diamond anvil [2,3] is of great importance for the analysis of condensed inert gases under extreme conditions; in this method the inert gas inside a diamond cell is compressed to the pressures of around a million atmospheres [4–8]. These pressures include a transition from attration to repulsion of atoms — closest neighbors. The subject of study in this paper is the analysis of behavior of inert gases in a phase line of fusion in the area of transition from attraction to repulsion of atoms. This transition occurs at pressures of around a hundred thousand atmospheres, i. e. is within the area of the experimental capabilities.

Therefore, the subject of the subsequent analysis — condensed inert gas, is a system of weakly interacting atoms, i. e. a wave function of atomic valence electrons is distorted lightly through interaction of atoms and therefore interaction of a test atom with the surrounding atoms hardly depends on the configuration of other atoms. Taking this into account and relating the mechanical and thermodynamic description of this system of interacting atoms with the experiment results, we obtain the full description of the considered system of atoms. In this article we express pressure and temperature, i. e. thermodynamic parameters, via the parameters of the pair potential of atom interaction. In particular, this leads to fewer jumps of entropy and density in process of a phase transition as the average atom interaction changes from attraction to repulsion. Besides, in the changing point as such, relying on the experimental data, we relate the pressure and temperature to the average distance between the atoms in the condensed inert gas.

2. Pair potential of inert gas atom interaction

In virtue of the repulsive nature of the potential of exchange interaction of inert gas atoms in the condensed inert gas the atoms maintain their individuality, i. e. parameters of atoms therein hardly differ from their values for an isolated atom, and the distance between the closest neighbors is great compared to the atom size. Therefore, the properties of the condensed inert gas depend on the potential of pairwise interaction of atoms.



Potential of pairwise interaction of atoms $U(R)$ as function of distance R between them [10]. Here R_e, D — parameters of the minimum potential of atom interaction, R_0, r_o — distances between the atoms, when the potential of the pairwise interaction of the atoms is equal to zero and 0.3 eV accordingly.

It is convenient to present the potential of interaction between two identical atoms of inert gas as a function of distance R between the atoms in the generalized Sutton–Chen form [9]

$$U(R) = D\left[\left(\frac{R_e}{R}\right)^{2n} - 2\left(\frac{R_e}{R}\right)^{n}\right]. \quad (1)$$

Presentation of the interaction potential in the analytical form is convenient for its practical application. As you can see, the potential of interaction of (1) two atoms of inert gas presented in the figure includes both the area of the potential well and the area of atom repulsion. The parameters of interaction potential of two inert gas atoms in the area of the minimum (R_e, D), contained in Table 1, were restored in papers [10–14] from the processing of the data related to the spectra of diatomic molecules of inert gases, differential and full scattering sections in atom collision, to the second viral coefficient of inert gases, and to the parameters of crystalline inert gases. These parameters are given in Table 1 and will be used further.

The data in the field of atom repulsion, where the potential of atom interaction substantially exceeds the dissociation energy of a diatomic molecule D, was obtained from processing of experimental results on thermal conductivity of inert gases [15,16]. The experimental capabilities also define the upper border for the repulsion potential, which is compliant with the maximum temperature of inert gases equal to 5000 K. This temperature is compliant with the energy of interaction at the border of the considered interval at approximately 0.36 eV. Thermal conductivity of inert gases at this temperature used to find the energy of atom repulsion is given in Table 1.

Let us imagine the nature of potential restoration for the pairwise potential of inert atom interaction on the basis of the measured thermal conductivity coefficients in the inert gas. The thermal conductivity coefficient of monoatomic gas κ, which is defined by elastic collisions of atoms, in the first approximation of Chapman–Enskog is given as the following expression [17,18]

$$\kappa = \frac{25\sqrt{\pi T}}{32\sqrt{m}\cdot\Omega^{(2,2)}}, \quad \Omega^{(2,2)} = \int_0^\infty t^2 e^{-t}\sigma^2(g)dt,$$

$$t = \frac{mg^2}{4T}, \quad \sigma_2(g) = \int (1-\cos^2\theta)d\sigma, \quad (2)$$

where T — temperature expressed in energy units, m — mass of atoms, g — relative speed of colliding atoms, θ — scattering angle. In this case the repulsive potential of interaction radically decreases as the distance between the atoms increases. At the same time, in accordance with the used Chapman–Enskog method [17,18], which is expansion in moments, i.e. the numerical parameter, the following members of the expansion contribute approximately 4% to the thermal conductivity coefficient. Atom scattering in this case complies with the model of solid spheres, where the potential of atom interaction is characterized by an infinite potential well. Taking into account the actual potential of interaction, which sharply depends on the distance between the atoms in the field that defines thermal conductivity, let us imagine the considered moment in atom scattering as [19,20]:

$$\Omega^{(2,2)} = \frac{2}{3}\pi R_t^2, \quad U(R_t) = 0.83T. \quad (3)$$

In the end formula (3) is expansion in a small parameter that characterizes the sharp change in the potential of atom interaction. This sharpness is described with a small parameter $1/k$, if the potential of atom interaction at the considered distance between the atoms is approximated by dependence $U(R) \sim R^{-k}$, besides, formula (3) takes into account the first two members of expansion by this small parameter. Therefore, the precision of this approximation is several percents.

To build the potential of inert gas atom interaction in the form (1) we use the experimental values of thermal conductivity of inert gases at temperature 5000 K [15,16], the precision of which is defined as 4%. The values of the corresponding thermal conductivity coefficients κ at temperature 5000 K are given in Table 1, as the values of the used small parameter of expansion α at this temperature, which is introduced as

$$\alpha = \left(\frac{d\ln\kappa(T)}{d\ln T} - \frac{1}{2}\right)^{1/2}. \quad (4)$$

Table 1 contains also the parameters of pair potential of inert gas atom interaction presented in the form (1). As you can see, this potential of interaction is close to the Lennard–Jones potential [21]. Table 1 contains the values of the distance between the atoms r, when the potential of interaction is equal to $U(r) = 0.36$ eV, and also the distances between the atoms R_0, when the potential of interaction passes through zero $U(R_0) = 0$.

Table 1. Parameters of pair potential of inert gas atom interaction

Atoms	Ne	Ar	Kr	Xe
D, meV	3.6	12	17	24
R_e, A	3.09	3.78	4.01	4.36
α	0.16	0.19	0.10	0.25
$\kappa(5000\,\mathrm{K})$, 0.01 W/(m K)	30.5	12.7	7.53	4.79
r, Å	2.07	2.72	2.92	3.27
n	6.0	5.8	5.5	5.6
R_0, Å	2.75	3.33	3.53	3.85

3. Behavior of dense inert gas in the phase line of fusion

It seems that the behavior of the considered physical object, which is a system of atoms with pairwise interaction of atoms — closest neighbors, may be analyzed on the basis of state-of-the-art computer equipment by method of molecular dynamics. This would make it possible to establish a connection between the mechanical and thermodynamic properties of the system However, such approach turns out to be dead-end in virtue of the specific behavior of this system. Indeed, the change in the configuration of atoms occurs as a result of transfer of barrier transitions between the local minima of the system [22,23], so a noticeable change in the configuration of atoms requires too much time.

Therefore, the connection between the mechanical and thermodynamic properties of the considered systems of atoms is established as a result of averaging of the individual atom motion based on the method described in [24]. This leads to the equation of state [25], which connects the pressure and temperature with the potential of atom interaction. In particular, for the inert gas crystal, when the interaction between the closest neighbors is taken into account, the equation of state is [26]:

$$p = \frac{T}{V(a)} + P(a),\ V(a) = \frac{a^3}{\sqrt{2}},\ P(a) = \frac{4a}{V(a)}\left|\frac{dU(a)}{da}\right|. \tag{5}$$

where p — pressure, T — temperature, V — volume per one atom, a — distance between the closest neighbors of the crystal, $U(a)$ — potential of the pairwise interaction of atoms at the distance of a between them.

Let us consider the behavior of the condensed inert gas near the phase line of fusion. Having limited ourselves to the interaction between the closest neighbors, we will describe every aggregate state, solid and fluid, by two parameters, namely, average distances between the closest neighbors a_s and a_l for the solid and liquid states, and also the average occupation numbers γ_s and γ_l for these states. According to the definition of the occupation number, the average number of the closest neighbors γ for a sample atom is $q = 12\gamma$. In these parameters the equations of state (5) for the solid and liquid states are as follows

$$p = \frac{\gamma_s T}{V(a_s)} + \gamma_s^2 P(a_s), \quad p = \frac{\gamma_l T}{V(a_l)} + \gamma_l^2 P(a_l). \tag{6}$$

Besides, the parameters included in formula (6) are defined in formula (5).

In addition to the equations of state in the phase line of pressure the Clapeyron–Clasius equation [27,28], which within the used approximation takes the following form

$$\frac{dp}{dT} = \frac{\Delta Q}{T\Delta V}, \quad \Delta Q = 6\gamma_l U(a_l) - 6\gamma_s U(a_s),$$

$$\Delta V = \frac{V(a_l)}{\gamma_l} - \frac{V(a_s)}{\gamma_s}. \tag{7}$$

Here ΔQ — specific heat spent for fusion, and ΔQ — change in the specific volume (volume per single atom) in fusion. The obtained equations make it possible to analyze the conditions that support the actual nature of fusion.

Considering the phase transition in the condensed inert gases, we follow the general principles of physics of aggregate states [29]. The liquid and solid aggregate states are the ones that are characterized by short-range order, therefore, the average distances between the test atom and its closest neighbors are close. Long-range order, which is valid as a result of interaction between the neighbors who are more distant, specifies the crystalline structure of the atoms in the solid state. In case of a condensed inert gas at low temperatures the internal energy is defined by the interaction of the closest neighbors, as it follows from the comparison of the internal energy of crystals [30] with the energy of interaction of the closest neighbors. The obtained conclusion on the small contribution of interaction between more distant neighbors to the internal energy of this system of interacting atoms covers a wider area of temperatures and pressures. Then the solid and liquid aggregate states are described similarly.

Let us rewrite the equations of state (6) as equations for pressure and temperature

$$p = \frac{\gamma_s V(a_s)P(a_s) - \gamma_l V(a_l)P(a_l)}{V(a_l)/\gamma_l - V(a_s)/\gamma_s},$$

$$T = \frac{\gamma_s^2 P(a_s) - \gamma_l^2 P(a_l)}{\gamma_s/V(a_s) - \gamma_l/V(a_l)}. \tag{8}$$

To analyze the behavior of the condensed inert gas in the phase line of fusion within the considered model together with equations (7) and (8), we use the experimental data for the position of the phase line of fusion. In process of fusion in the area of atom attraction the volume per one atom increases, since the phase transition from the solid state with the crystalline structure of atoms, i. e. ordered distribution of atoms in the space changes into the liquid state with the chaotic distribution of atoms. At the same time the fusion is characterized by absorption of heat, i. e. in process of fusion the conditions are met in the area of atom attraction

$$\Delta V > 0, \quad \Delta Q > 0. \tag{9}$$

In accordance with the Clapeyron–Clausius (7) equation, this corresponds to the pressure increase with temperature in the phase line of fusion in the area of atom attraction.

When crossing the changing point R_0, so that $U(R_0) = 0$, the first condition (9) is met, since the chaotic distribution of atoms requires higher density of atoms compared to the ordered ones under the same conditions. The second condition (9) may be violated, and depending on the preservation or violation of these conditions, the nature of the behavior after passing the changing point may vary [31]. However, the experimental data shows that the pressure in the phase line of fusion increases with the growth of temperature, i. e. fusion conditions (7) stay in the area of atom repulsion.

Let us imagine the criteria that provide for the compliance with the conditions (7). Let us introduce the parameters

$$\Delta = \frac{a_s - a_l}{a_s}, \quad \delta = \gamma_s - \gamma_l. \tag{10}$$

In accordance with the general principles of physics of aggregate states [30] the parameter Δ is small. Then in the triple point $\gamma_s = 0.94$ and $\gamma_l = 0.80$. Let us introduce the parameter

$$\xi = \frac{\gamma_s \Delta}{\delta}. \tag{11}$$

Further within the used approximation we will express the considered physical values via this parameter, considering parameters (10) small and expanding in them. Then equations (8) will have the following form:

$$p = \frac{\xi\gamma_s^2 w(a_s) - \gamma_s^2 P(a_s)}{1 - 3\xi}, \quad w(a_s) = -\frac{d[a_s^3 P(a_s)]}{a_s^2 da_s}.$$

$$T = \frac{k_1 V(a_s)[\xi\gamma_s v(a_s) - 2P(a_s)]}{1 - 3\xi}, \; v(a_s) = -a_s\frac{dP(a_s)}{da_s}. \tag{12}$$

Here the specific volume V is in Å^3, values p, P, w, v are expressed in GPa, and temperature T is in K. The coefficient of conversion between these values is $k_1 = 72.5\,\mathrm{K/(Å^3 \cdot GPa)}$. Besides, the values u and U are expressed in meV. Besides, the Clapeyron–Clasius equation (7) in the new variables will take the following form

$$\frac{dp}{dT} = \frac{6k_2[\xi\gamma_s^2 u(a_s) - \gamma_s^2 U(a_s)]}{TV(a_s)(1 - 3\xi)}, \; u(a_s) = -a_s\frac{dU(a_s)}{da_s}, \tag{13}$$

besides, the coefficient of conversion of measurement units is equal to $k_2 = 0.16\,\mathrm{GPa \cdot Å^3/meV}$. The experimental dependence of pressure on temperature on the phase line of fusion is added to these equations.

Therefore, equations (12) and (13) together with the experimental dependence $p(T)$ in the phase line of fusion relate thermodynamic parameters p and T with mechanical parameters a_s and γ_s, expressing them via the value ξ, which in accordance with formula (11) is the parameter of the changing point $a_s \approx R_0$, where $U(R_0) = 0$. As you can see, the presented equations provide a full description of the condensed inert gas in the phase line of fusion near the changing point within the used model at the specified potential of interaction of two inert gas atoms. Table 2 provides the values that define the properties of condensed inert gases in the phase line of fusion near the changing point of atom interaction from attraction to repulsion.

Table 2. Values describing the behavior of the condensed inert gases in the phase line of fusion, near the changing point from attraction to repulsion of atoms

Atoms	Ne	Ar	Kr	Xe
R_0, Å	2.75	3.33	3.53	3.85
$P(R_0)$, GPa	3.8	6.8	7.8	8.6
$w(R_0)$, GPa	520	1300	1600	2200
$v(R_0)$, GPa	80	140	150	170
$u(R_0)$, meV	87	280	350	550
ξ, %	15	10	9.5	7.9
$p(R_0)$, GPa	3.2	5.5	6.2	6.8
$T(R_0)$, 1000 K	0.5	0.7	0.9	1.3

Table 2 provides the values included into formulas (12) and (13) in the point of atom interaction sign change. Therefore, we obtain the conditions imposed onto the value of parameter ξ, which have the following form

$$\frac{1}{3} > \xi > 0.1.$$

The left part of this condition ($\xi < 1/3$) meets the requirement that in fusion the density of atoms increases. The other part of this condition proceeds from the requirement that the values of pressure and temperature remain the positive values.

Based on the data of Table 2 it is possible to simplify the ratios between the thermodynamic parameters of the condensed inert gas in the vicinity of the changing point. In particular, here we receive the ratio of pressure to temperature in this area, which does not depend on parameter ξ:

$$\frac{p}{T} = \frac{\gamma_s w(R_0)}{v(R_0)V(R_0)}. \tag{14}$$

Here you can find the contribution of the thermal motion of atoms to pressure p based on the equation of state (6), which is equal to

$$\xi(R_0) = \frac{\gamma_s T(R_0)}{V(R_0)p(R_0)} = \frac{w(R_0)}{v(R_0)}. \tag{15}$$

These values for the condensed inert gases near the changing point are given in Table 2. Based on these values and the equation of state (6), we find the pressure in the atom interaction changing point on the phase line of fusion according to formula

$$p(R_0) = \frac{\gamma_s^2 P(R_0)}{1 - \xi(R_0)}. \quad (16)$$

These values are listed in Table 2. By combining them with the experimental data for dependence $p(T)$, let us define the temperature in the atom interaction changing point. Note low accuracy of this operation, since the used data is available in the graphic form and is obtained by approximation of data from the area of lower temperatures, where the object temperature is fixed, and also from the area of higher temperatures, where the object temperature is determined on the basis of the object radiation in the infrared area of the spectrum. Besides, the experimental dependences of pressure on temperature $p(T)$ on the phase line of fusion were used, which were presented in paper [32] for neon, in paper [33] for argon and crypton, and also in papers [33,34] for xenon.

The parameter γ_s, being the ratio of the average number of the closest neighbors for the internal atom to 12, i. e. to the corresponding number of the closest neighbors in the crystal, deserves special attention. The values of this parameter for the solid and liquid states of inert gas when the interaction changing point is approached on the phase line of fusion try to come near. Obviously, the area of this parameter values at each temperature is narrow in virtue of the requirement that at the considered temperature this parameter, on the one hand, was related to the condition with the chaotic distribution of atoms in the space, and, on the other hand, was compliant with their ordered distribution in the crystal. Note that in the triple point the value of this parameter for the solid state is 0.94, and for the liquid one it is equal to approximately 0.80 [1,35]. Obviously, we will not be seriously mistaken if the accept the value of this parameter in the interaction changing point on the phase line of fusion as equal to $\gamma_s = 0.85$. The accuracy of pressure and temperature values in Table 2 in the atom interaction changing point on the phase line of fusion is estimated at (30−40)%.

4. Conclusion

In analysis of condensed inert gases we combine the mechanical properties of these systems, using the potential of interacting atoms as classic particles, their thermodynamic properties, describing the solid and liquid aggregate states with temperature and pressure, and the experimental data. Besides, the potential of interaction between the atoms is of pairwise nature, and according to the measurements, the primary contribution to the inner energy of the crystal is made by interaction between the closest neighbors. The model used in the paper is based on this concept and takes into account the interaction between the closest neighbors. This model was used to consider the behavior of condensed inert gases in the phase line of fusion in the vicinity of the changing point of atom interaction from attraction to repulsion.

The short-range order model makes it possible to express the thermodynamic parameters of condensed inert gases in the fusion line via the parameters of the atom interaction parameters. Even though this does not provide a full description of the considered system of atoms even when the experimental fusion line is used, however, it makes it possible to relate the thermodynamic parameters, pressure and temperature, with the average distance between the closest neighbors. Moreover, it follows from here that in a motion from a triple point to the area of transition from attraction to repulsion along the phase line of fusion, the jumps of entropy and density decrease and become much smaller when they enter into the changing area compared to those in the triple point.

In the atom attraction area the fusion of solid inert gas is accompanied with the atom density growth and heat absorption. Atom density also increases in process of fusion in the atom repulsion area, since fusion is a transition from the ordered distribution of atoms in space to the chaotic one. The change of the inner energy in process of fusion in the atom repulsion area could have had any sign, but according to the experiment, the pressure in the phase line of fusion increases along with temperature. Therefore, according to the experimental data and Clapeyron−Clasius equation the fusion of the solid inert gas in the atom repulsion area is accompanied with heat absorption.

The feature of the motion in the atom interaction changing point in the phase line of fusion is the decrease in the jump of atom density and inner energy as the changing point is approached. Within the used model, with account of interaction between the closest neighbors, criteria were received, under which the change of inner energy in process of fusion maintains its sign when passing through the changing point. Also note that the accounting for only the short-range order for the solid state of inert gas, which is fair according to the experimental data away from the changing point, is disturbed when this point is approached. Nevertheless, other conclusions remain.

It is substantial that the pressure resulting in the transition from attraction to repulsion is several GPa for solid inert gases, whereas the diamond anvil method makes it possible to do the measurements up to the pressure of approximately 100 GPa. Therefore, the transition of inert gas from atom attraction to repulsion is available for experimental analysis by the diamond anvil method. As for the phase transition between the solid and liquid aggregate states of inert gas, i. e. fusion, it tends to the second-order phase transition when approaching the atom interaction changing point, even though it remains the first-order phase transition [36].

Note another aspect of this study. One of its objectives was to build a potential of interaction between the two identical atoms of inert gas, starting from the bottom of the potential well and to the shorter distances between the atoms up to strong repulsion. Even though the dependence of atom interaction potential on distance R between the atoms is approximated by a combination of power-law functions $1/R$, this is not of principal importance, and it may be approximated by exponential dependences. The accuracy of the obtained atom interaction potential is estimated to be 20%. The conventional method to determine the inert gas atom interaction potential in the area of repulsion is based on the analysis of differential cross section of fast atom scattering into small angles, but the accuracy of this method is estimated by the coefficient of order 2. It seems that the most accurate method could have been based on the measurements of dependence on pressure for a specific volume found from the analysis of Bragg scattering of X-ray radiation on a highly compressed inert gas, where the accuracy of measurement of each value is estimated at several percent. However, in the case of neon, the potentials of interaction in the area of strong repulsion obtained from the data on thermal conductivity and parameters of strong atom compression, differ almost twice [37]. These deviations between the interaction potentials may be explained by the absence of thermodynamic equilibrium in a strongly compressed neon. Nevertheless, the studies of the inert gas in the phase line of fusion at high pressures is of interest both for understanding the behavior of inert gases under extreme conditions, and for analysis of the potential of pairwise interaction of atoms.

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Conflict of interest

The authors declare that they have no conflict of interest.

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