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The Study of the Molecular Diffusion in Gases and Liquids

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Abstract: The molecular dynamics calculations of the velocity autocorrelation functions and the diffusion coefficients for argon and krypton atoms in argon have been carried out. The data of the molecular dynamics simulations are analyzed to understand the change of the diffusion mechanism with transition from dense gas to liquid. In dense gases, the diffusion mechanism is the same as in rarefied gases, and the temperature dependences of the diffusion coefficient are alike. A new diffusion mechanism appears in liquids. This diffusion mechanism isn't connected with the jumping motion of the molecules. Probably, it is connected with the motion of the molecules group surrounding a molecule. Then the velocity of the molecule is relaxed with the decreasing of the average velocity of the molecules group. Various structures of the systems within the vapor – liquid phase transition region have been found and investigated. A comparison of the simulation results with the experimental data on diffusion in gaseous and liquid argon yields good agreement.

Keywords: Diffusion, Gases and liquids, Molecular dynamics method

Introduction

Mathematical description of the molecular diffusion in gases and liquids has long been a problem of the physical kinetics, studing transport processes (diffusion, viscosity, thermal conductivity, etc.). Though the research in this field has been conducted more than a hunred years, the problem still is far from being solved. There is a good kinetic theory of molecular diffusion in rarefied gases based on the solution of Bolzman's equation by Chapman – Enskog method, (Chapman & Cowling, 1952; Hirschfelder, Curtiss & Bird, 1964). Things are worse with the theory of diffusion in dense gases and liquids. It is related with the fact, that the diffusion mechanisms in thse media are studied not well enough. The existing theoretical models (Ferziger & Kaper, 1972; Frenkel, 1955) often bring to unsatisfactory results. In such situation the direct numeric simulation methods and the molecular dynamics method developed by Alder & Wainwright (1959, 1960) and Rahman (1964), are very useful.

The molecular dynamics method has long been applied for the calculations of the diffusion coefficients. In papers Alder, Gass & Wainwright (1970), and Erpenbeck & Wood (1991), the self-diffusion coefficients in hard absolutely smooth elastic spheres model have been calculated. In papers, Erpenbeck (1989, 1992, 1993), the diffusion coefficients in hard spheres mixtures have been calculated. In papers Heyes (1988), Meier et al. (2004) and Laghaei et al. (2006), the systems of particles interacting by Lennard-Jones potential has been studied. Other laws of interaction have also been used Liu, Silva & Macedo (1998), and Dubrovin et al. (2002). In our papers, Zhilkin & Kharlamov (2015), Kharlamov & Zhilkin (2016, 2017), the dependances of the diffusion coefficients in gases and liquids on density and temperature at the conditions of phase transition vapour – liquid have been reseached. In papers Kharlamov (2018 and 2021), the change of the diffusion mechanism has been detected as a result of transition from dense gases to liquids. At the same time it is shown that the diffusion mechanism in liquids is not related with the jumps of the molecules from one quasi-stationary state to another, and is determined, more likely, by the collective movement of the group of molecules surrounding some picked out molecule (Kharlamov, 2023 and 2024). In present paper the survey of the results acquired in this field is proposed.

Method

The calculations of the diffusion coefficients have been made for two systems, in wich the particles interact according to the Lennard-Jones potentials. The first system (system 1) consists of identical particles, the second (system 2) – of two different types of particles. The content of the second type particles constitutes 1 % of the whole quantity of the particles in the cell of the molecular dynamics method. The whole number of particles is from 3000 to 40000.

In our investigations the Lennard-Jones pair potential is used. The cutting of the potential takes place at a distance $r = 5\sigma_c$ with the help of the cubic spline.

$$\begin{aligned} &U(r) = 4\varepsilon_i\left[\left(\frac{\sigma_i}{r}\right)^{12} - \left(\frac{\sigma_i}{r}\right)^{6}\right],\ r \le 4.5\sigma_c, \\ &U(r) = a_i\left(r-5\sigma_i\right)^2 + b_i\left(r-5\sigma_i\right)^3,\ 4.5\sigma_c \le r \le 5\sigma_c, \\ &U(r) = 0,\ r > 5\sigma_c. \end{aligned} \tag{1}$$

The subscript *i* takes value 1 for the particles of the first type, value 2 for the particles of the second type and value 12 for the potential of the first and second type particles interacting with each other. The parameters a_i and b_i are chosen according to the conditions of the Lennard-Jones potential equality and its derivative and the corresponding values of the spline at $r = 4.5\sigma_c$. This potential provides the absence of the particles interaction at long distances ($r > 5\sigma_c$). At the same time such way of the potential cutting leads to the smooth dependance and makes the calculations in the molecular dynamics method more accurate. In our calculations the dimensionless variables are used:

distance $r = r_d/\sigma_1$;
time $t = t_d/\sigma_1\,(\varepsilon_1/m_1)^{1/2}$;
density $\rho = \rho_d\,\sigma_1^3$;
temperature $T = k\,T_d/\varepsilon_1$;
energy $U = U_d/\varepsilon_1$.

σ_1, ε_1, m_1 are the parameters of the Lennard-Jones potential and the mass of the first type particles. Low index *d* marks the dimentional variables.

The following parameters of the Lennard-Jones interaction potential are used:

for the first type particles ε_1/k = 124 K and σ_1 = 3.418 Å ;
for the second type particles ε_2/k = 190 K and σ_2 = 3.609 Å ;
for the first and second type particles ε_{12}/k = 153.5 K and σ_{12} = 3.514 Å .

The chosen parameters of the Lennard-Jones potentials correspond to argon and krypton atoms (NIST Chemistry WebBook). The cutting of the potentials in formula (1) is carried out at $\sigma_c = \sigma_2$. The relation of the krypton and argon atoms masses equals m_2/m_1 = 2.098. The applied algorithm of the molecular dynamics method is described in details in (Kharlamov & Zhilkin, 2017, April 20).

The Calculations of Velocity Autocorrelation Functions and the Diffusion Coefficients

After the system comes to equilibrium the time dependence of the velocity autocorrelation functions (VACF) of the first and second type particles is calculated

$$F(t)=\frac{\langle \vec{\mathrm{v}}(0)\cdot\vec{\mathrm{v}}(t)\rangle}{\langle \mathrm{v}^2(0)\rangle}=\frac{\sum_{j=1}^{n}\vec{\mathrm{v}}_j(0)\cdot\vec{\mathrm{v}}_j(t)}{\sum_{j=1}^{n}\mathrm{v}_j^2(0)}\,. \tag{2}$$

Here $\vec{\mathrm{v}}_j(t)$ is a particle velocity at time moment *t*. Then the diffusion coefficients D_{md} are calculated by the Green – Kubo formula:

$$D_{md}=\frac{kT}{m_{1,2}}\int_0^\infty F(t)\,dt\,. \tag{3}$$

For the comparison of the acquired results with the theoretical data the reduced self-diffusion coefficients D_{md}/D_0 for the first type particles – the argon atoms and the diffusion coefficients D_{md}/D_{12} for the second type particles – the krypton atoms in argon are calculated. Here

$$D_0=\frac{3\sqrt{\pi m_1 kT}}{8m_1\rho\pi\sigma_{11}^2\Omega^{(1,1)*}}\,,$$
$$D_{12}=\frac{3\sqrt{2\pi m_{12}kT}}{16m_{12}\rho\pi\sigma_{12}^2\Omega^{(1,1)*}} \tag{4}$$

the Chapman – Enskog diffusion coefficients in the kinetic theory of rarified gases (Hirschfelder, Curtiss & Bird, 1964). The dimensionless density takes values: ρ = 0.00349; 0.0348; 0.1; 0.4; 0.437; 0.61; 0.78; 0.84 and 0.88. The dimensionless temperature varied over the range from 0.6 to 6.

Results and Discussion

First of all, it should be noted, that the calculation results of the velocity autocorrelation functions and the diffusion coefficients are qualitatively alike for these two systems (system 1 and system 2). It means that the diffusion mechanisms in both systems are identical under the same conditions of density and temperature. As a whole, as far as density is concerned we can conventionally divide all the systems under consideration into three states: low density systems – rarified gases ($\rho < 0.1$), middle density systems – dense gases ($0.1 \le \rho \le 0.61$) and high density systems – liquids ($\rho > 0.61$). Let us examine each of these states separately.

The Low Density Systems

Let us consider the calculation results of these systems in the example of system 2. In figure (Figure 1) the distribution of the krypton atom in argon at a low system temperature is presented. We can see random even distribution of the krypton atoms in the cell. In figure (Figure 2) the krypton atoms velocity autocorrelation function of this system is shown. It is an exponential curve according to the Boltzmann – Chapman – Enskog theory of rarified gas (Hirschfelder, Curtiss & Bird, 1964). In figure (Figure 3) the temperature dependence of the diffusion coefficients of the krypton atoms in argon at density ρ = 0,00349 is demonstrated. This dependence is in accordance with the rarified gases theory and corresponds to formula (4). This dependence is the power law $D \sim T^{0.86}$ (Kharlamov, 2024).

The diffusion coefficients, which we calculate by the molecular dynamics method, are in good agreement with the experimental data. In paper (Durbin & Kobayashi, 1962) the experimental data on the diffusion of the krypton admixture in gasious argon is presented. For example, at argon density ρ_d = $14.67\cdot10^{-3}$ g/cm^3 and temperature T_d = 308.1 K the experimental diffusion coefficient D_{exp} = $1.563\cdot10^{-3}$ cm^2/s, and for density ρ_d = $40.136\cdot10^{-3}$ g/cm^3 – D_{exp} = $0.5701\cdot10^{-3}$ cm^2/s. Our calculations show values $1.563\cdot10^{-3}$ cm^2/s and $0.5694\cdot10^{-3}$ cm^2/s correspondingly. The same good agreement is observed for the diffusion coefficients in gaseous argon (Winn, 1950) and krypton at low pressure (Codastefano et al., 1978). The comparison of our self-diffusion coefficients calculation results in argon is presented in paper (Kharlamov, 2023). Here is the comparison of our calculations results with the experimental data for the coefficients of self-diffusion in gaseous krypton at the low pressures (Codastefano et al., 1978). For example, at temperature T_d = 293 K and density ρ_d = 35.19·10^{-3} g/cm^3 the self-diffusion coefficient equals D_{exp} = 0.9717·10^{-2} cm^2/s, and at density ρ_d = 113.3·10^{-3} g/cm^3 – D_{exp} = 0.2929·10^{-3} cm^2/s. Our calculations show the values 1.0835·10^{-2} cm^2/s and 0.2824·10^{-3} cm^2/s correspondingly.

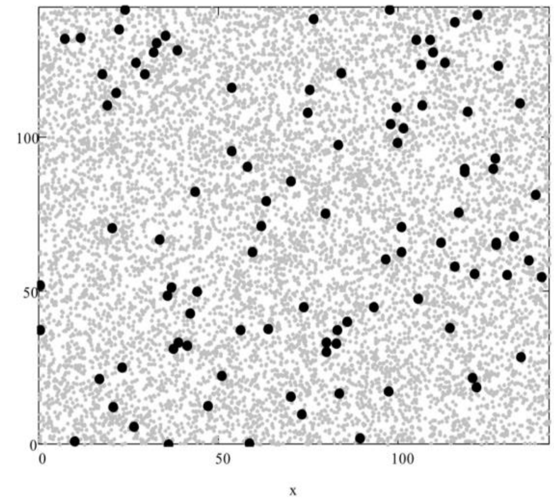

Figure 1. Snapshot of particle distribution in the cell at ρ = 0,00349 and T = 0,75. The small dots are the positions of the argon atoms, bold dots are the positions of the krypton atoms

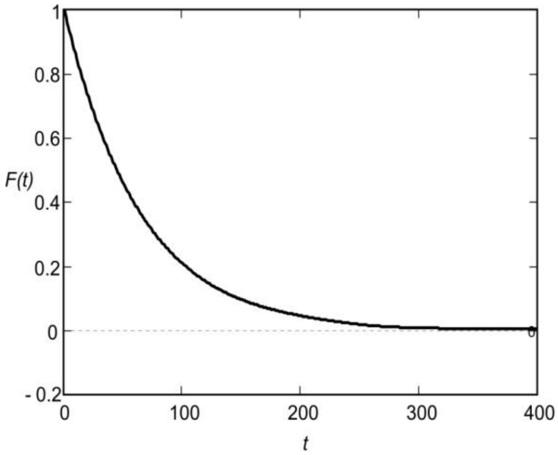

Figure 2. Velocity autocorrelation function of krypton atoms in argon (ρ = 0,00349; T = 0,75)

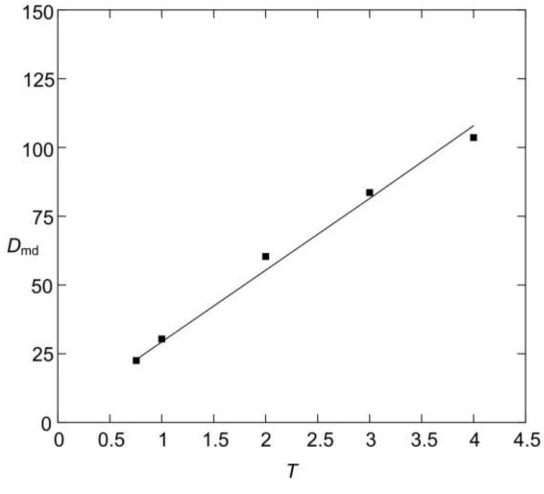

Figure 3. Temperature dependence of the diffusion coefficient D_{md} for the krypton atoms in argon at the system densities ρ = 0.00349. The solid curve is the linear fit

The Middle Density Systems

In the systems of middle density the phase transision vapor – liquid is observed at low temperatures ($T < 2$). In this case the formation of nanodrops in gas (Figure 4, a), bubbles of gas in liquids (Figure 4, b), layering of the system into gas and liquid is possible (Zhilkin & Kharlamov, 2015), (Kharlamov & Zhilkin, 2017). Nanodrops, which are formed in vapor as a result of homogeneous nucleation, have unusual thermodynamic properties. For example, the notion of surface tension can not be used for them (Kharlamov et al., 2008), (Kharlamov et al., 2010), (Kharlamov et al., 2011), (Kharlamov et al., 2012). It is also established, that the krypton atoms are captured by such nanodrops, so that an increased concentration of krypton is observed inside the drops (Kharlamov, 2021).

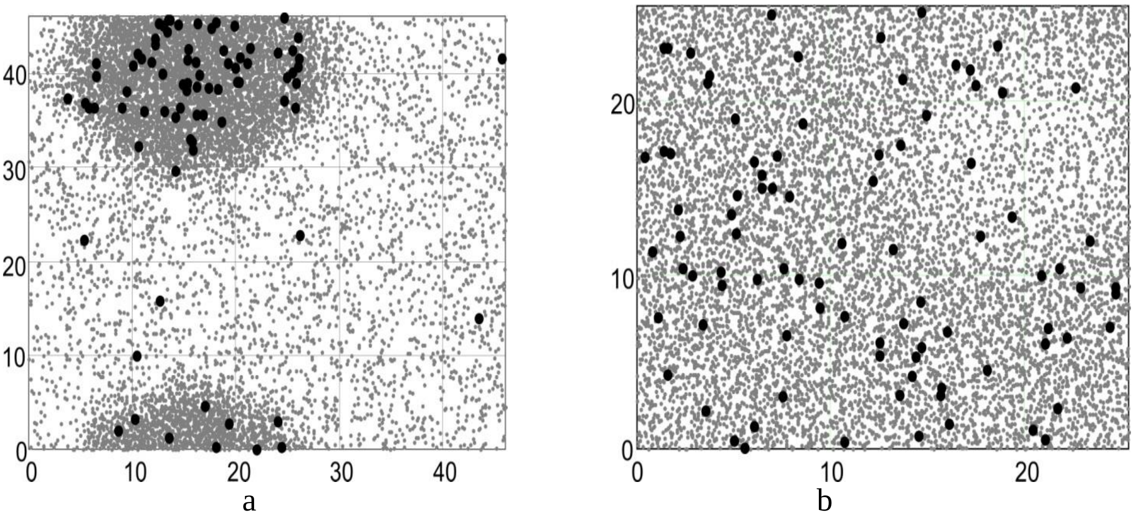

Figure 4. Snapshots of particle distribution in the cell at $\rho = 0.1$, $T = 1$ (a) and $\rho = 0.61$, $T = 1$(b). The small dots are the positions of the argon atoms, bold dots are the positions of the krypton atoms

At high temperatures ($T \geq 2$) the homogeneous distribution of argon and krypton density is observed for such systems. In figure (Figure 5) the time dependence of the velocity autocorrelation function of krypton atoms in argon is presented. It is not exponential with a long power tail ~ $t^{-3/2}$ (Kharlamov, 2023), which was discovered earlier in the papers (Rahman, 1964), (Alder et al., 1970).

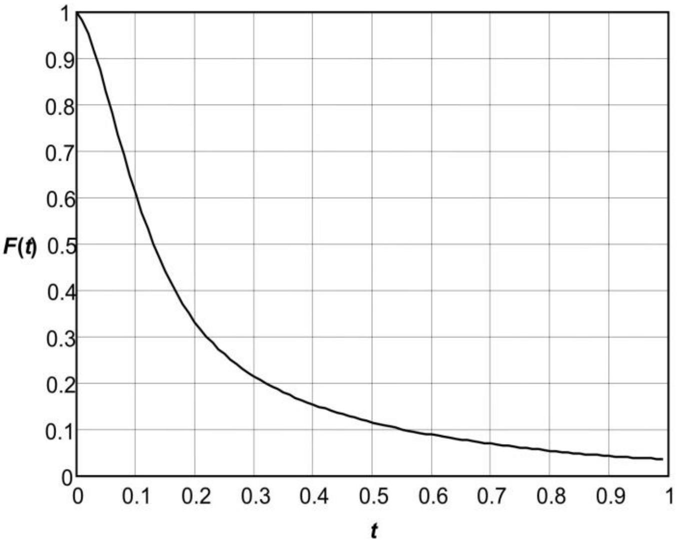

Figure 5. VACF of the krypton in argon at the system density $\rho = 0.61$ at the temperature $T = 2$

In Figure 6, the dependence of the diffusion coefficients of the krypton atoms in argon on density at various temperatures is shown. One can see that the reduced diffusion coefficients D_{md}/D_{12} do not depend on temperature, and depend only on density for the systems of low and middle density ($\rho < 0.61$). It testifies that the diffusion mechanism for these systems is the same. The relaxation of the krypton atoms velocity in this case takes place in general due to the pair collisions of these atoms with the argon atoms. Such diffusion mechanism we called “collisioning” (Kharlamov, 2018). The dependence approximation of the calculated diffusion coefficients on density leads to the expression:

$$f_d = \frac{D_{md}}{D_{12}} = 1 - 0.210\rho - 0.257\rho^2 - 0.244\rho^3 . \tag{5}$$

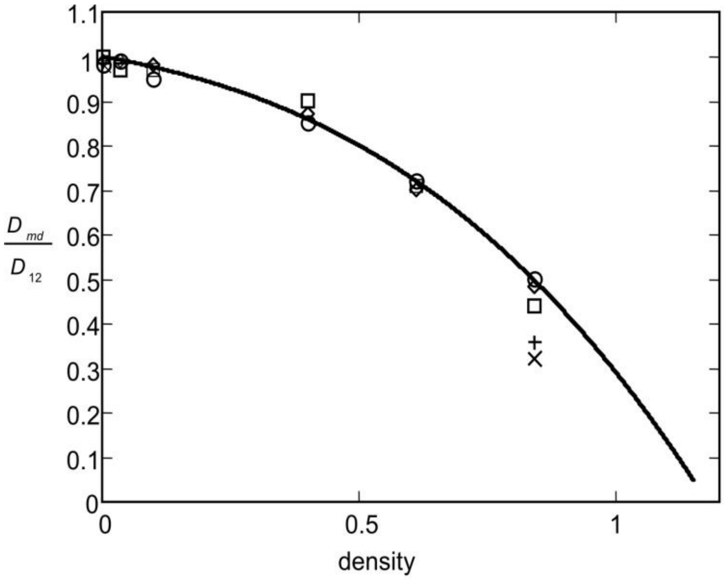

Figure 6. Density dependences of the reduced diffusion coefficients D_{md}/D_{12} at different system temperatures: T = 0.75 (×), T = 1 (+), T = 2 (□), T = 3 (◊), T = 4 (○).

Analogous results are received for the dependences of the self-diffusion coefficients in gaseous and liquid argon (system 1). In this case the approximation curve of this dependence has the form (Kharlamov & Zhilkin, 2017, April 20):

$$f_{sd} = \frac{D_{md}}{D_0} = 1 - 0.547\rho + 0.3\rho^2 - 0.574\rho^3 . \tag{6}$$

Expressions (5) and (6) are the universal dependences of the diffusion coefficients on the density for the rarified and dense gases. The comparison of our calculation results and the experimental data in the middle density systems is carried out in paper (Kharlamov, 2023). A satisfactory agreement is proved for the diffusion coefficients in dense gaseous argon (Mifflin & Bennet, 1958).

The High Density Systems

In Figure 7, the typical time dependence of the velocity autocorrelation function of the argon atoms in liquid argon is presented. It has the characteristic negative tail, which testifies about the return atom movement in the liquid in the definite time interval. The reduced diffusion coefficient for such systems depends not only on density, but also on temperature (Figure 6). More so, the dependence of the diffusion coefficient on the temperature in liquids is close to the linear one (Figure 8). The approximation of the calculated coefficients by the linear dependence leads to the expression

$$D_{md} = -0.0132 + 0.0688 \cdot T . \tag{7}$$

So, we can see, that the diffusion mechanism in liquids differ from that in dense gases. It is related with the fact, that in liquids the collective effects are of importance. Apparently, in this case separate atoms move surrounded by a group of neighboring atoms, doing damped vibrations inside the group. The atom velocity relaxation is defined by the average velocity relaxation in this group. At the same time such diffusion mechanism is not "jumping", because in this case the temperature dependence of the diffusion coefficient must obey the Arrhenius equation (Frenkel, 1955)

$$D = D_m \, e^{-\frac{\Delta W}{kT}} \, . \tag{8}$$

The comparison of the experimental data on the diffusion of argon atoms in liquid argon (Cini-Castagnoli & Ricci, 1960, July 13), (Cini-Castagnoli & Ricci, 1960, December 30), and also on diffusion of krypton atoms in liquid argon (Cini-Castagnoli & Ricci, 1960, December 30; Dunlop & Bignell, 1998) lead to a satisfactory agreement (Kharlamov, 2023).

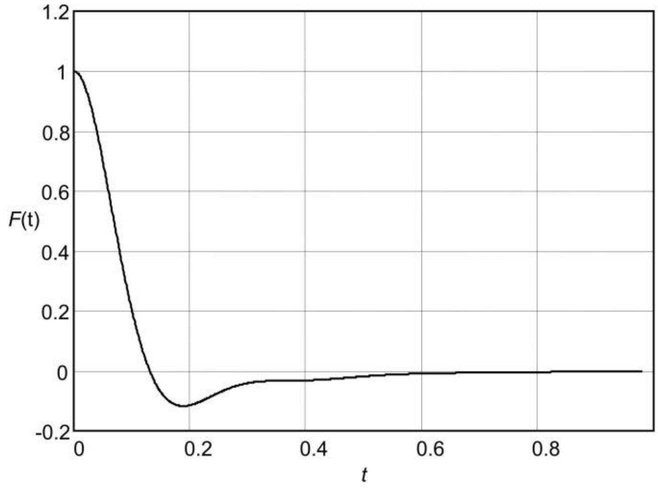

Figure 7. VACF of argon atoms in argon at the system density ρ = 0.84 at the temperature T = 0.75

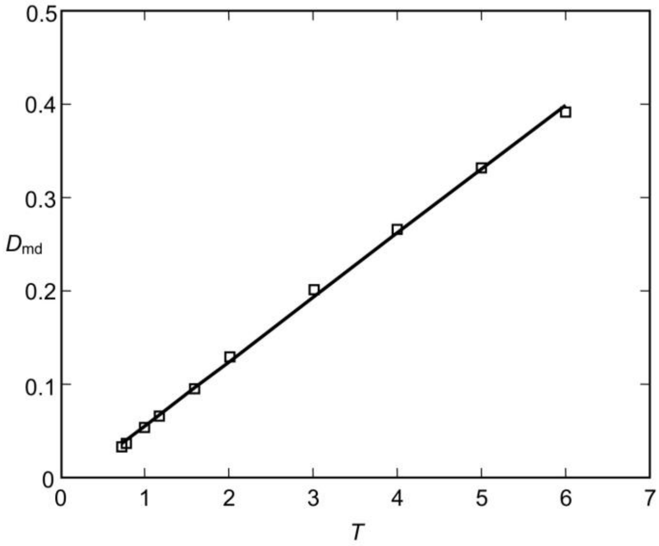

Figure 8. Temperature dependence of the diffusion coefficient D_{md} for the argon at the system densities ρ = 0.84. The solid curve is the fit (7)

Conclusion

Thus, we see that the molecular dynamics method gives good results in the calculations of the diffusion coefficients not only in liquids and dense gases, but also in rarified gases. It permits to calculate the diffusion coefficients with the accuracy of the experiment, as well as to reveal subtle details of the diffusion phenomenon, such as the diffusion mechanisms and the relaxation of the molecular velocity. It also allows observing the phase transition vapor – liquid and its influence on the diffusion of an admixture in the binary molecular system.

The special problem of the diffusion theory is the study of the diffusion mechanisms of nanoparticles and macromolecules in liquids and gases. And though in this field we obtained some interesting results (Rudyak, Kharlamov & Belkin, 2000, September 3; Rudyak et al., 2000; Rudyak et al., 2001), the problem is far from being solved completely. Another important problem of the gases and liquids theory, which we work on, is the problem of study of the big density, momentum and energy fluctuations (Rudyak & Kharlamov, 2003; Kharlamov & Rudyak 2004). It is especially important in connection with the phase transitions vapor – liquid in the systems under consideration. One more interesting task is the simulation of the light-induced drift in rarified gases. Though the simplest theory of this phenomenon has been created in a whole (Gel'mukhanov et al., 1992), there are still numerous unrevealed things in the mechanism of this phenomenon.

Recommendations

The fulfilled research has not only the fundamental scientific character, but also possesses the applied potential. It can be used in the calculations of the chemical and thermo physical processes in industrial technologies.

Scientific Ethics Declaration

The author declares that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the author.

Acknowledgements or Notes

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