



SCIREA Journal of Physics

ISSN: 2706-8862

<http://www.scirea.org/journal/Physics>

December 20, 2024

Volume 9, Issue 6, December 2024

<https://doi.org/10.54647/physics140663>

Influence of the Conservation Angular Momentum Law and the mathematical models for Continuum Mechanics and Kinetics

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Abstract

The most common systems are open non-equilibrium non-stationary systems. From the previously formulated equations and some experiments, the connection between the gradients of physical quantities and the moment of momentum (force) is traced. The main equations of the theory are the Liouville equation, constructed on the basis of Hamilton's theory for closed systems, and the equations constructed using it. The article investigates some processes from this trace. The use of the Hamiltonian formalism and the dependence of the force only on the distance between particles limit the study. In the collision integral, for example, for a rarefied gas, the Lennard-Jones potential is often used, which is not of the type considered. The foregoing forces us to turn to the study of the influence of forces of a more general form on the equations of mechanics. Hamilton's formalism traces the behavior of closed systems. The general form of boundary conditions and forces changes the theory proposed in the works by N.N. Bogolyubov. The results of the reformulation are discussed. Even in classical theory,

after taking moments, we arrive at Boltzmann's theory at no symmetric stress tensor. The symmetric tensor is obtained after the assumption of a small effect of no symmetry and from the condition of the balance of forces. The requirement of simultaneous fulfillment of the laws of conservation of forces and moments of forces leads to the existence of two solutions. To take into account the angular momentum, in addition to the conditions for the equilibrium of forces, the law of equilibrium of the moments of forces is required in the calculations. From it, the degree of no symmetry of the stress tensor is determined. In previous works the contribution of the distributed moment of force illustrate to the problems of continuum mechanics and the kinetic theory. Examples of the solution to the problem of fluid mechanics, the theory of elasticity and kinetic theory were given early. Here we discuss the theory needed to account for the lack of symmetry of the stress tensor.

Keywords: equations and boundary conditions, kinetic theory., the influence of the angular momentum, dislocation, vacancies.

1. Introduction.

The most general open non-stationary systems, which are objects of research in continuum mechanics and kinetics, are considered. Mathematical modeling of such objects causes difficulties, since their description is represented by a system of non-linear non-stationary equations. In previous works it was shown that classical models do not include one of the most important laws - the law of conservation of angular momentum, if the moment does not act as a given force action. The performed mathematical analysis of the equations of continuum mechanics with the initial asymmetric stress tensor showed that in the plane case for four unknowns in the classical formulation we have three equations: two equations from the stress equilibrium condition and one equation - the moment equilibrium condition. Thus, we need to close the problem with the help of an additional condition. In the classical version, such a condition is the stress tensor symmetry condition [1-6].

It does not follow from the definition of pressure, both from the classical Boltzmann equation and from the modified one, that the hydrostatic pressure is one third of the sum of the pressures on the coordinate areas. Using Pascal's law for equilibrium, the pressure is chosen equal to one third of the pressures on the coordinate areas. However, the theory remains the

same when determining different pressures on each of the areas, i. e. p_x, p_y, p_z [7]. Using one pressure is possible under equilibrium conditions (Pascal's law), but for nonequilibrium conditions this fact is not obvious. Neglect of the extra-integral term when taking integrals by parts (Ostrogradsky-Gauss theorem) is possible only for slow laminar flows. The difference in pressure is indicated by the analysis of the determination of pressures when comparing the results of its determination through potential velocities by substitution into the Euler equations. Writing down the equilibrium law separately for forces and separately for moments of forces without taking into account their mutual influence, although the moment creates an additional force, we come to the conclusion about the symmetry of the stress tensor. In the case where we consider equal pressures in different directions, we lose the moment of force, and the gradient of the moment is the force. Experiments have shown, in particular, that the inviscid vortices that carry the energy of the main fluctuations (known in part as vortices from the inertial range) are small, with a size comparable to the thickness of the boundary layer. This means that the derivatives of the velocity pulsations with respect to coordinate and time are large compared to the derivatives of the averaged velocity profile with respect to the longitudinal evolution coordinate. Nevertheless, averaging procedures are applied that exclude these large terms from the equations. As a result, any closure hypothesis reduces the TPS equations to an averaged simplified analogue of the laminar parabolic equations of motion [8]. When estimating the values, it is also necessary to take into account the fact that, according to experiments, the Kolmogorov and Landau-Lifshitz theories, most of the kinetic energy of pulsations in the TPS is contained in fast inviscid vortices, the characteristic dimensions of which are of the same order along all coordinate axes and are comparable with the thickness of the boundary layer. Analyzing the results of solving the Euler equations and calculating potential flows, we obtain a vortex sheet, which indicates the existence of a momentum, calculations [9-11]. The proof of the correctness of the theoretical representation of the equations of continuum is verified in two ways. One way is to represent physical quantities through the sum of delta functions, The second way is to calculate all physical quantities by solving the Boltzmann equation or another kinetic equation and taking the corresponding moments representing the physical quantities being calculated.

The Boltzmann equation is obtained using the Liouville equation, which in turn is based on the Hamiltonian formalism [12-14]. Closed systems are considered. When deriving, only the interaction of individual particles is always taken into account, so the symmetry of the force potentials is assumed. The potential considered in the theory corresponds to the dependence

$\Phi(r_i - r_j)$, r_i, r_j the radii of the molecules. Real forces have more complex components. An example of other forces is, for example, the Lennard-Jones potential. It is often used in calculating the collision integral. In this case, we can talk about the discrepancy between the Boltzmann equations obtained from the classical Liouville equation, which is widely used. Consideration of stochastic equations based on the sum of two integrals and the concept of a physically infinitesimal scale leads to the effect of additional diffusion. The vector nature of the pressure was previously proven by studying the equations for the potential flow and through the distribution function.

For macroparameters, the balance equation is written in integral form, after which the integral is taken by parts, neglecting the term outside the integral [7]. However, interactions are not only individual in nature, but also collective interactions have a great influence. A similar situation is observed in quantum mechanics. The whole does not behave as a sum of its parts. The behavior of each part changes in the presence of other objects. Due to the cumulative nature of interaction effects, the properties of the system can differ significantly from the properties of individual components. The influence of collective effects is especially strong for charged particles. Since computational methods are currently widely used to obtain a solution, the article discusses the accuracy of the numerical solution obtained for the distribution function and by the molecular dynamics method. The flow method or its variants are often used to calculate the equations of continuum mechanics. It is important to remember that the equations obtained by the flow method do not correspond to the experimentally obtained equations, since they are based on a symmetric stress tensor. The article briefly discusses these issues.

2. Hamiltonian dynamics

The class of systems considered in textbooks on statistical mechanics includes systems described by Hamiltonian dynamics. In the modern version, this class includes all systems described by the laws of classical or quantum mechanics. Since the theory we propose assigns an important role to the law of conservation of momentum (momentum), it is necessary to study how the properties and structure of the system will change when using the law of conservation of momentum, since it has not been considered in statistical theories. We have already noted that a feature of classical theories is the identification of the properties of systems without studying the influence of boundary and initial conditions on their state.

Usually, the Hamiltonian contains only potential forces. In reality, the forces are represented by the sum of forces (q-generalized coordinates) [15]

$$\begin{aligned} Q &= -B - Cq, \quad \dot{q}_i = 0, \quad B \\ &= D + \Gamma, \quad D^T = D, \quad \Gamma^T \\ &= -\Gamma, \end{aligned}$$

Dq-dissipative, *Gq*-gyroscopic, *C*-potential.

$$\begin{aligned} -\Gamma\dot{q} &= \frac{d}{dt} \frac{\partial V}{\partial \dot{q}} - \frac{\partial V}{\partial q}, \\ V(q, \dot{q}) &= -\frac{1}{2} q^T \Gamma q. \end{aligned}$$

The matrix of potential forces *C* is also the sum of symmetric and no symmetric forces:

$$C = K + N, \quad K^T = K, \quad N^T = -N.$$

Conservative forces have the potential

$$-Kq = \frac{\partial U}{\partial q}, \quad U = -\frac{1}{2} q^T K q.$$

Therefore, $L = T - Q_r$, where the last term is the generalized forces. Formally, we can write the formula of the classical

$$\dot{q}_i = \frac{\partial H(q, \dot{q})}{\partial \dot{q}_i}, \quad \ddot{q}_i = -\frac{\partial H(q, \dot{q})}{\partial q_i}.$$

However, they often work with more general forces.

$$(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n) = (q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n, p_{l+1}, \dots, p_n), \quad p_k = \frac{\partial T}{\partial \dot{q}_k}$$

$$H = \sum_{1 \leq i \leq N} \left(\frac{p_i^2}{2m} + U(r_i, t) \right) + \frac{1}{2} \sum_{1 \leq i, j \leq N, i \neq j} \Phi(|r_i - r_j|).$$

Often

$$\Phi = \left(\frac{a}{r^6} - \frac{b}{r^{12}} \right), \quad \frac{\partial \Phi}{\partial r} = -6 \frac{a}{r^7} + 12 \frac{b}{r^{13}}.$$

Then the result is the sum of two potentials, the system does not belong to the Hamiltonian system.

In the equilibrium state, the distribution function for practical applications represents two cases:

1. An isolated system, when the total energy of the system has some given value.
2. A system in a thermostat.[13].

It is believed that using the microcanonical and canonical Gypsum distributions, various thermodynamic functions can be calculated. In this case, the temperature of the surrounding bodies is specified. For a nonequilibrium state in statistical mechanics for nonequilibrium processes, the Gypsum ensemble is proposed. It cannot be used for dynamic systems. In addition, the condition for its applicability is the conservation of the average energy of the system. It follows that the Gypsum distribution can only be used in the case of a small perturbation of energy in a selected small element in the classical formulation.

$$\left(\frac{\partial}{\partial t} + r_1 \frac{\partial}{\partial r_1} F_0(r_1) \frac{\partial}{\partial p_1}\right) f_1 = n \int \frac{\partial \Phi_{12}}{\partial r_1} \frac{\partial f_2}{\partial p_1} d r_2$$

$$\Phi_{ij} = \Phi(\varphi(i, j))$$

$$\left(\frac{\partial}{\partial t} + r_1 \frac{\partial}{\partial r_1} F_0(r_1) \frac{\partial}{\partial p_1}\right) f_1 = n \int \frac{\partial \varphi}{\partial r_1} \frac{\partial \Phi_{1i}}{\partial \varphi} \frac{\partial f_1}{\partial p_1} \prod_{\substack{ij \\ i \neq j}} d r_{ij}$$

$$\Phi_{ij} = \Phi(\varphi(r_{ij}))$$

For the simplest potentials, an iterative procedure can be constructed using the Hamiltonian formalism. It follows from the above that the theorem on conservation of phase volume for an arbitrary potential is not satisfied and the Jacobian of the transformation from current momenta to initial ones is not equal to unity. The collision cross section is usually calculated for the chosen potential, without changing the phase volume. However, estimates show that the product of the cross section by the corrected value of the phase volume remains close to unity. Otherwise, the product of the "correct" cross section and the phase volume gives either an overestimated or an underestimated value.

3. Boltzmann equation

When solving the Boltzmann equation by the Chapman-Enskog method, when taking the derivative of the locally equilibrium distribution function in the classical case, the Euler equations are used. The question arises about the legitimacy of using the parameters

determined from the Euler equation for the locally equilibrium distribution function. These parameters are determined from the zero approximation, and the problems are solved taking into account the first order, which corresponds to the solution of the Navier-Stokes equations. When taking the derivative of the distribution function, the number of particles is assumed to be constant, which excludes adsorption and variable density. As a result, the classical solution does not determine self-diffusion. A derivative of the form is considered

$$\frac{\partial f_0}{\partial t} \Big|_{t=0} = f_0 \left\{ \frac{m}{kT} \left(c_i c_j - \frac{1}{3} c^2 \delta_{ij} \right) \frac{\partial u_i}{\partial t} + \frac{1}{2T} \frac{\partial T}{\partial t} c_i \left[\left(\frac{m}{kT} \right) c^2 - 5 \right] \right\}.$$

For the function

$$f(t, \mathbf{x}, \xi) = f_0(t, \mathbf{x}, \xi) = n \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left\{ - \frac{m}{2kT} (\xi - \mathbf{u})^2 \right\}.$$

Taking into account the change in density

$$\frac{\partial f_0}{\partial t} \Big|_{t=0} = f_0 \left\{ \frac{1}{n} \frac{\partial n}{\partial x_i} c_i + \frac{m}{kT} \left(c_i c_j - \frac{1}{3} c^2 \delta_{ij} \right) \frac{\partial u_i}{\partial x_j} + \frac{1}{2T} \frac{\partial T}{\partial x_i} c_i \left[\left(\frac{m}{kT} \right) - 5 \right] \right\}.$$

The new term is responsible for self-diffusion. This entails a change in the density, velocity and temperature fluxes. The Chapman-Enskog solution should then have even in the classical case

$$f = f^{(1)} \left(1 + \epsilon \varphi^{(1)} \right), \quad \varphi^{(1)} = - C_i \frac{\partial n}{\partial x_i} - A_i \frac{\partial T}{\partial x_i} - B_{ij} \frac{\partial u_i}{\partial x_j}.$$

The coefficients C_i, A_i, B_{ij} are functions of c_i, n, T . $c_i = \xi_i - u, n, T$; is the gas-dynamic velocity, n is the particle density, T is the temperature. The obtained results confirm the equations obtained in the works of S.V. Vallander [16,17]. Supplementing the equation

$$\begin{aligned} & \text{with the influence of the moment for the distribution function, we obtain } f(t + dt, \mathbf{r} + \\ & \xi_i dt + \mathbf{r} \times \boldsymbol{\omega} dt, \xi_i + \mathbf{F}_i dt + \frac{\partial M}{\partial \mathbf{r}} dt) d\mathbf{r} d\xi_i + G_2(t + dt, \mathbf{r} + \xi_i dt + \mathbf{r} \times \boldsymbol{\omega} dt, \xi_i + \mathbf{F}_i dt + \\ & \frac{\partial M}{\partial \mathbf{r}} dt) = f(t, \mathbf{r}, \xi_i) d\mathbf{r} d\xi_i + G_1(t, \mathbf{r}, \xi_i) + \left(\frac{\partial f}{\partial t} \right)_{coll} dt. \end{aligned}$$

M is the moment associated with the collective interaction of particles as a result of the motion of the center of inertia during particle motion, G_1 and G_2 are the flows through the boundary. According to estimates, the contribution of the moment to the collision integral is a value of the next order. However, the main contribution to the correlation function is made by the moment included in the convective operator as a zero-order value. The contribution of the moment to the pressure is especially large for structural molecules and charged particles. The

original formulation of all stochastic processes is the closedness of volumes, there are no flows through the boundary, and the Boltzmann equation is written under such assumptions. The methodology remains the same for open systems. Naturally, with full consideration, the equations for macroparameters change. They were presented earlier for the phenomenological theory.

4. Formation of sliding conditions and adsorption layer.

Let us consider the classical Knudsen layer. About 38 percent of the number of molecules contained on the outer boundary will reach the surface. It is this number that we will consider at the boundary of our layer. Only a small part, possessing low energy, can be adsorbed on the surface. The number depends only on the temperature. The majority of the molecules will be reflected, approaching at a distance equal to the radius of interaction of the gas molecule and the surface. The distance depends on the interaction potential of the molecules. These molecules will return to the outer boundary. The mean free path is too large, the interactions of gas molecules with the wall occur at significantly The adsorption time of the main components of air, having an adsorption heat of 20 MJ/kmol , at room temperature is 10^{-10} s , and at liquid nitrogen temperature - 1 s. The equations for macroparameters obtained in the kinetic theory are applicable inside the region, but near the boundary it is necessary to know the interaction of the flow molecules with the surface. With incomplete information about the interaction, fictitious boundary conditions (slip conditions) corresponding to the boundary of the Knudsen layer are specified. The boundary conditions for the Navier-Stokes equations are the boundary conditions for velocity and temperature (at constant density). Here it is proposed to split the problem into two. For a rarefied gas, at least at low flow velocities, it is proposed to consider a thinner layer equal to several radii of interaction of molecules. shorter distances. Gas molecules inside a thin layer do not collide, but collide with surface molecules. The role of collective effects decreases. Having obtained the distribution function at the layer boundary, it is necessary to solve the Boltzmann equation in the layer from this boundary to the boundary of the Knudsen layer by the small parameter method using the Chapman-Enskog function. This can be done due to a small change in the distribution function over the mean free path. You can try to study the distribution function at the layer boundary, which is determined by the modified Chapman-Enskog function taking into account the change in the number of particles. The interaction process is determined by the interaction potentials of the gas flow and the molecules the solid surface and the effect of the moment on structured

surfaces is also taken into account. Molecules moving toward the wall must be divided into three groups: low-speed molecules that subsequently stick to the wall, medium-speed molecules that are reflected from the wall, and high-speed molecules that penetrate the wall. The boundaries of the ranges are determined by the accommodation energy for a specific gas and surface material and the velocity of the incident molecule. When solving the problem, it is necessary to remember that the interaction potential depends on the interplanar distance between the surface layer and the previous one, which depends on the orientation of the crystallographic surface. In many cases, the distance increases, which entails a change in the interaction potential. process of gas adsorption by the surface. Langmuir was the first to take collective interactions into account. For crystalline metals, the change in potential during adsorption was calculated under the assumption of interaction of molecules of the nearest neighbors. In this paper, the same assumption is used taking into account the moment. The purpose of the analysis is a theoretical study of the causes of gas slip near the surface. Usually, when determining the slip length, it is assumed that the distribution function on the surface has the form

$$f_r = f_r(0, \xi_x, \xi_y > 0, \xi_z) = n_r \left(\frac{h_r}{\pi}\right)^{\frac{3}{2}} e^{-h_r \xi^2}.$$

The formula is written under the assumption that the vertical and horizontal velocities are equal to zero. Here r is for reflected molecules,

$$h^\pm = \frac{m}{2kT^\pm}.$$

When calculating macroparameters on a surface, such as the number of particles

$$n(0) = \int_{\xi_y > 0} f_i d\xi + \int_{\xi_y < 0} f_r d\xi = \frac{n(0)}{2} + \frac{n_r}{2} + o\left(\epsilon \frac{df_0}{dy}\right).$$

The difference in the distribution function is apparently significant, since for reflected particles the vertical component of the velocity is zero under the condition of no flow, for incident particles the total velocity is taken, similarly for other macroparameters. Boundary condition for internal

decomposition is

$$n(0) = \int_{\xi_y > 0} \xi_y f_i d\xi + \int_{\xi_y < 0} \xi_y f_r d\xi = 0.$$

If we assume that there is no adsorption and the macrovelocity on the surface is zero, then a paradox arises due to the difference in velocities, which can be resolved only under the

assumption that the gas is stationary near the surface. The probabilities of the equilibrium distribution function on the surface on the right and on the left differ in magnitude. As a result, the number of falling particles and the probabilities of movement to the right and to the left differ. The number of falling particles is determined by the quantities [18,19]

$$v_{\pi} = \frac{nv_S}{2\sqrt{\pi}} \left\{ e^{\left(\frac{U_x}{v_S}\right)^2} + \sqrt{\pi} \frac{U_x}{v_S} \left[1 + \Phi\left(\frac{U_x}{v_S}\right) \right] \right\},$$

$$v_{\pi} = \frac{nv_S}{2\sqrt{\pi}} \left\{ e^{\left(\frac{U_x}{v_S}\right)^2} + \sqrt{\pi} \frac{U_x}{v_S} \left[1 - \Phi\left(\frac{U_x}{v_S}\right) \right] \right\}$$

Let us introduce the following notation: v_{π} is the number of falling gas

molecules, v_S is the most probable velocity of gas molecules. The difference in the probability values v_S leads to the probability of directed motion along the inner boundary. In addition, two different forces arise during the interaction: one along the surface, the second vertically to the surface. The lattice parameters of aluminum are 4.050 Å. Under normal conditions, interacting with atmospheric oxygen, aluminum is covered with a thin (2-10⁻⁵ cm) film. Oscillating changes in the interplanar distance at the surface are about 10 percent or less (depending on the temperature and the face: loose or close-packed). For example, it is known that for tungsten at room temperature, the root-mean-square displacement of an atom from the equilibrium position is $\sigma < 0.1$ Å.

Phonon motion should not affect adsorption processes, with the exception of long-wave phonons, since the displacement of surface atoms is 0.1 ÷ 0.5 Å. During inelastic interaction of gas and photons, part of the gas energy is spent on excitation of phonons in the direction perpendicular to the surface, which corresponds to the process of flow scattering. Creation of a forest does not allow gas and phonons to interact. In addition, contact with the solid body is reduced. However, the processes of scattering of atoms and molecules occur differently for small and large irregularities and depend on the roughness height, since the contribution of the moment changes. The effect of slippage is enhanced by the moment arising from the difference in vertical and horizontal forces. The moment creates a force acting upwards or downwards. The moment participates in the growth of the forest.

5. Effect of torque on a crystalline body with a vacancy.

The strength of crystalline bodies is determined not only by the potentials between metal molecules, but also by the presence of vacancies and impurities inside the metal. It is known that dislocations are formed around impurities and vacancies and depend on the ratio of the masses of impurity and main atoms. The role of torque in the multiple distribution of impurities is theoretically analyzed. It is shown that, in addition, the new lattice structure depends on the difference in the interaction potentials of the lattice potential and impurity atoms with the main component. With a large positive difference, loosening of the structure near the impurity is observed, and with close arrangement of impurities, vacancies can form. Experimentally determined critical shear stresses for pure metals are several orders of magnitude lower than theoretically determined ones. Taking into account structural defects leads to closer theoretical results. A mechanism for the formation of new structures in a crystalline material associated with the action of a force with a distributed moment is proposed. The methods of elasticity theory, oriented to one-dimensional measurements, cannot be a source of information for determining the origin of dislocations and cracks. Moment effects are three-dimensional and have a collective nature. In the simplest case, they are two-dimensional with additional consideration of the force action of the third component. The conditions of formation and origin of cracks are associated with the influence of torque even in the equilibrium case. The effect of stresses aggravates the consequences. In the state of equilibrium, the force action of the moment, as compensating, can be calculated, knowing the distribution of forces near the defect.

In the mathematical theory of plasticity, hardening and fracture, experimental data are taken as initial data. The theory of elasticity is more developed, but even in the region of low stresses it is not possible to explain some effects. The physical mechanism is not studied in such theories. During plastic deformation, the appearance of anisotropy is observed, that is, the acquisition of different mechanical properties in different directions [20-22]. There are no ideal crystal lattices. The formation of dislocations near the surface and deep in the material occurs in different ways. Apparently, forces act near the surface, ensuring that, under the influence of loads, the defect reaches the surface and the formation of short dislocations. The role of the moment is insignificant if you do not take into account the processes of accommodation. Experimentally determined critical shear stresses for pure metals are several orders of magnitude lower than theoretically determined ones. Taking into account structural defects leads to closer theoretical results.

The movement of phonons should not affect the adsorption processes, with the exception of the case of long-wave phonons, since the displacement of surface atoms is 0.1÷0.5 Å. In the inelastic interaction of gas and photons, part of the gas energy is spent on excitation of phonons in the direction perpendicular to the surface, which corresponds to the process of flux dissipation. Creating a forest prevents gas and phonons from interacting. In addition, contact with solid particles is reduced. However, the processes of scattering of atoms and molecules occur differently for small and large irregularities and depend on the height of the roughness, since the contribution of the moment changes. The sliding effect is enhanced by the moment arising from the difference between vertical and horizontal forces. Moment creates a force that acts up or down. We theoretically analyze the role of torque in multiple impurity distribution. It is shown that, in addition, the new lattice structure depends on the difference in the potentials of interaction between the lattice potential and the impurity atoms with the main component. With a large positive difference, loosening of the structure near the impurity is observed, and with close proximity of impurities, the formation of vacancies is possible. Experimentally determined critical shear stresses for pure metals are several orders of magnitude lower than theoretically determined ones. Taking into account structural defects leads to closer theoretical results. Let us consider the initial stage of dislocation formation. Let there be a vacancy inside the material. In equilibrium, the forces arising from lattice distortion are not sufficient to move molecules. Let there be free space near the border. For the Lennard-Jones potential

$$F(a) = -4\varepsilon \left[-12 \frac{\sigma^{12}}{a^{13}} + 6 \frac{\sigma^6}{a^7} \right],$$

$$F(2a) = F(2a) + 4 F(a\sqrt{2}) + 4 \cdot F(2a\sqrt{2}),$$

$$F = 0 = F(2a) + 12F(a\sqrt{2}) =$$

$$= -4\varepsilon \left[-12 \frac{\sigma^{12}}{(2a)^{13}} + 6 \frac{\sigma^6}{(2a)^7} \right] - 12 \left\{ -4\varepsilon \left[-12 \frac{\sigma^{12}}{(a\sqrt{2})^{13}} + 6 \frac{\sigma^6}{(a\sqrt{2})^7} \right] \right\},$$

$$\mathbf{F}(\mathbf{r} + \Delta\mathbf{r}) = -4\varepsilon \left[-12 \frac{\sigma^{12}}{(\mathbf{r} + \Delta\mathbf{r})^{13}} + 6 \frac{\sigma^6}{(\mathbf{r} + \Delta\mathbf{r})^7} \right].$$

From the equation you can determine the equilibrium point r_0 . Full force

$$F_c = F + \gamma, \quad \gamma - \text{stresses acting on one molecule.}$$

Let us consider the relationship between the forces of the “correct” and distorted lattices.

$$\varphi = \frac{-4\varepsilon\left[-12\frac{\sigma^{12}}{(2a)^{13}} + 6\frac{\sigma^6}{(2a)^7}\right]}{-4\varepsilon\left[-12\frac{\sigma^{12}}{a^{13}} + 6\frac{\sigma^6}{a^7}\right]} \approx 0.008.$$

The moments from each vacancy will intersect and exert additional force on the middle molecule, causing it to move, increasing the distance between the vertically positioned molecules. In the presence of a large number of defects, the moments will add up, resulting in the formation of an area of increased concentration of vacancies (pores). Various transition regimes may exist near the surface. The role of surface effects is important. For liquids near a smooth surface, a model with a thin layer of stationary liquid can be proposed. The width of the layer is determined by the magnitude of dynamic friction (an analogue of turbulent flow). Internuclear O–H distances are close to 0.1 nm, the distance between the nuclei of hydrogen atoms is 0.15 nm, and the angle between H–O–H bonds is 104.5°. The minimum distance between aluminum molecules is $L = 3.1038 \text{ \AA}$, the size of water molecules is $r_0 = 31.8 \text{ \AA}$, the mean free path is $\gamma = 21.6 \div 36.6$, the cluster size is $9.06 \div 1.22 \text{ nm}$. [23]. Some molecules are in a free state. It is these molecules that carry out transport processes in liquids. The size ratio indicates the possible overlap of the gaps between surface molecules by a water molecule. For capillaries with a radius on the order of the cluster radius, sliding is possible due to contact with the wall of a small part of the cluster.

6. Conclusion

In the work, investigations were continued to refine the equations of a continuous medium and the Boltzmann equation taking into account the angular momentum as result of moving molecules. The positions of the kinetic theory that lead to the symmetry of the stress tensor are investigated in classic case. The article discusses mathematical models of the rarefied gas kinetic theory, conditions for the formation of sliding and adsorption layers. Previous work shows that classical models do not include one of the most important laws - the law of conservation of angular momentum if the moment does not act as a given force. A feature of classical theories is the identification of the properties of systems without studying the influence of boundary and initial conditions on their state. Now the main apparatus is the Hamiltonian formalism. In the modern version, all systems described by the laws of classical or quantum mechanics belong to the class of Hamiltonian systems. The features of such systems related to the openness of the systems, boundary conditions, and type of potential are

discussed. The use of Hamilton's formalism and the dependence of the force, which depends only on the distance between particles, limits classical studies. In the collision integral, for example, for a rarefied gas, the Lennard-Jones potential, which is not related to Hamiltonian systems, is often used. Improved Chapman-Enskog solution for open system.

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