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ABSTRACT

of the dissertation for the degree
of Doctor of Philosophy

**PHENOMENOLOGICAL STUDY OF NANO PHENOMENA
IN PSEUDOPOTENTIAL NEWTONIAN LIQUIDS**

Specialty: 2206.01- Molecular Physics

Field of science: Physics

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BAKU - 2022

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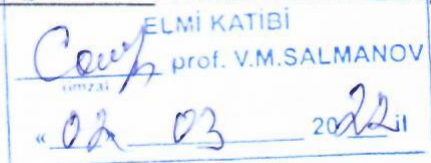


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GENERAL CHARACTERISTICS OF WORK

Relevance and currency of the research topic. One of the most important scientific and practical issues in the condensed matter physics is surface phenomena. So many processes and events are significantly related to these phenomena – capillarity, wetting, fluidity in liquids and etc., melting, phase formation, equilibrium of intermediate phases in the second type of superconductors in solids etc.

Processes that occur at the boundary (surface) of the separation of two phases is characteristic and differs significantly from the corresponding volume processes. The phases in contact are separated from each other by a narrow layer that differs significantly from the structure of homogeneous phases due to their atomic (molecular) structure. In the special case, the average distance between atoms (molecules) in the subsurface layer is about 10% larger than the intermolecular distance. The density of particles in the subsurface layer changes according to a non-monotonous, complex law as it moves away from the surface to the volume. As in surface tension, the viscosity of liquids is the result of direct intermolecular interactions between adjacent fluid layers, approximately a few nanometers thick. These phenomena can be called nanophenomena.

One of the main specific parameters characterizing surface events is the surface tension coefficient (σ). Physically, this quantity is the free energy of the unit separation surface, that is, the work required to change the surface isothermally into a unit. All thermodynamic quantities that characterize a surface are related to the surface tension coefficient, in other words, it is important to know the surface tension to determine them.

The dependence of surface tension and viscosity on various physical and chemical factors has been extensively studied by various authors for more than a hundred years. However, for a wide range of liquids, there is no universal approach or theory, at least in terms of quality. The main difficulty in creating an appropriate microscopic theory is related to the complex structure of the subsurface layer and the inability to select the potential for intermolecular interactions.

Relevant experimental results with existing microscopic theories often differ by up to 40%, according to the value of σ . The latter shows the futility of microscopic theories.

There are many empirical or semi-empirical relations and expressions for surface tension and viscosity in the literature. However, they are offered for a limited temperature range or for certain classes of liquids. Therefore, taking into account the above, it can be concluded that one of the most important issues in fluid physics (as well as molecular physics) is to determine the law of surface tension and viscosity of liquids over a wide temperature range, in other words, which allows us to describe nanoparticles and is suitable for all liquids (except exotic liquids).

Research objects and subjects. Liquids of various natures (mainly metallic liquids) were taken as the object of research.

The purpose and duties of the research: Phenomenological determination of analytical regularity of nanoparticles with surface tension and viscosity in pseudopotential Newtonian fluids and to investigate the possibility of a correlation between these phenomena.

In order to achieve this goal, the following issues will be studied in detail:

- Essential study of the mechanisms of viscosity and surface tension in normal Newtonian fluids;
- Specificity of dynamic viscosity and surface tension in liquid metals;
- To determine the general (universal) expression of the dynamic viscosity of Newtonian fluid from the phenomenological point of view and its application to liquid alkali metals;
- To determine the universal analytical regularity of the surface tension of liquids from the phenomenological point of view and to consider in detail the issue mentioned in the example of alkali metal liquids;
- In metallic liquids to study the possibility of separate assessment of dynamic viscosity of ionic and electron aggregates;
- To study the possibility of correlation between the phenomena of viscosity, surface tension and self-diffusion in liquid metals.

Research methods. The method of thermodynamics and potentials is used as research methods in the dissertation. Based on these methods, the relationship between surface tension and dynamic viscosity for alkali metal fluids and their temperature dependence were determined.

The main provisions of the defense.

1. The surface tension and dynamic viscosity of liquids are related to the presence of a surface layer, which is determined by the effect of intermolecular interactions occurring in the physical layer and since the thickness of this layer is in the nanometer order, both events can be identified as nanoparticles.

2. The regularities determined using the methods of thermodynamics and potentials for surface tension and dynamic viscosity of alkali metal fluids correctly describe a wide range of temperatures.

3. The hydrodynamic model cannot be applied to alkali metal fluids, and the Stokes-Einstein relationship is unsuitable for these fluids, ie self-diffusion and dynamic viscosity occur by different mechanisms - due to diffusion density fluctuations, and viscosity under the influence of force.

4. Since the liquid metal is a specific binary solution, so it is a system of free electrons and ions, and the viscosity of the liquid metal consists of the sum of the accumulations of ions and electrons, and is $\eta_i \approx 10\eta_e, \eta_i \sim T^{-2} \forall \eta_e = const.$

5. Dynamic viscosity to high temperatures not too close to the boiling point is a non-activation process, and it occurs by the transport of phonons within the nanolayer and the kinetic movement of free electrons.

6. A correlation has been established between the dynamic viscosity of liquid metals and the coefficient of surface tension, and based on this correlation it is possible to calculate the energy of intermolecular communication in liquids.

7. Surface tension and dynamic viscosity are not like a macroscopic molecular transfer event, but a nano event that is established in a surface layer of several angstroms.

8. There is a relationship between the coefficient of surface

tension and the coefficients of thermal compression and expansion, and based on this, the thickness of the surface layer can be estimated and decreases with increasing temperature.

Scientific innovation of research.

1. Based on the analysis of the method of potentials (or cycles), practically, determination of regularities that accurately describe the surface tension and dynamic viscosity of liquids up to boiling point;

2. Determination of analytical dependence at two arbitrary temperatures in liquids according to the density value which allows to calculate the temperature heat of surface formation (formation) at temperatures $T < T_b$;

3. To determine the correlation between surface formation and molecular weight and Fermi energy for alkali metal fluids;

4. To determine the relationship between the volume and surface properties of alkali metal fluids and to evaluate the thickness of the subsurface layer based on this relationship;

5. Proposal (development) of the method of separation of ionic and electronic components of dynamic viscosity of liquid metals and its application to several liquids;

6. The unsuitability of the Stokes-Einstein relation for alkali metal fluids between the self-diffusion coefficient and the dynamic viscosity;

7. To determine that the dynamic viscosity in normal liquids at low temperatures is a non-activation process - it is directly related to the phonon transitions between adjacent nano layers.

Theoretical and practical significance of the research. The value of the results obtained from a practical point of view the proposed new method allows to study the nano properties of liquids up to temperatures close to the critical temperature. This is especially valuable for toxic liquids and high temperature areas. The results obtained in the dissertation can also be useful in the development of the theory of fluids (the kinetic theory).

Approbation and application. The main provisions and results of the dissertation were discussed at the following conferences and published in their materials:1) BSU, Institute of Physics, 2014,

№3 (Conference); 2) International Republican Conference, Baku: 2014; 3) XXXV International Correspondence Scientific-Practical Conference “Scientific discussion: questions of mathematics, physics, chemistry, biology”, 2015; 4) BSU Actual Problems, Baku: 2015; 5) IV International Scientific Conference of Young Researchers, Qafqaz University, 2016; 6) XVIII Republican Scientific Conference, Baku: BSU, 2016; 7) V International Scientific-Practical Conference “Modern Problems of Metal Physics” Baku: June 10-11, 2016; 8) “International Conference: Modern Trends in Physics” BSU, Baku-2017, April 20-22; 9) “II International Congress of Scientific Research”, Ankara, 2020, March 6-8;

The materials of the dissertation were published in 14 articles (1 of them in journals indexed in the Web of Science) and 9 theses in local and foreign journals.

Name of the organization where the dissertation work is executed. It was performed at the National Aerospace Agency at the Institute of Space Research of Natural Resources.

Structure, volume and main content of dissertation work. The dissertation consists of 147 pages - introduction, 4 chapters, results, 31 tables, 19 figures and a list of 211 used scientific literature. The volume of the dissertation (excluding gaps and pictures in the text, tables, graphs and bibliography) - 136360 characters (introduction - 12224, Chapter I - 40125, Chapter II - 22321, Chapter III - 35351, Chapter IV - 24141, result - 2198 characters).

The first chapter is devoted to the analysis and generalization of various models and approaches to the surface tension and structure of fluids. It has been shown that existing theories and models of the structure of fluids often contradict experimental results. Both the hole model and the quasi-crystalline model are only qualitatively suitable for liquids of limited class and limited physical conditions. The free surface of liquids leads to surface phenomena. In the first chapter of the dissertation an extensive literature review has been provided on this issue. For this purpose, the relevant results obtained from static, dynamic methods,

thermodynamic (including quasi-thermodynamic) and statistical mechanics methods were mutually analyzed. It has been shown that the methods established from the 1890s (by Van der Waals, Laplace, Ray, etc.) have not essentially changed until recent years, and it is semi-hypothetical.

The first chapter examines in detail the atomic (molecular) structure of the surface layer, as well as the regularity of the possible distribution of density. As explained in this chapter, the phenomenon of surface tension is due to molecular processes in the nanometer-thick surface layer. For this reason, of course, it can be considered a nanophenomenon.

Neutronographic and X-ray studies show that each liquid molecule has an atomic coverage similar to that of a sparse but mobile crystalline structure. According to these ideas, liquids have a close atomic (molecular) arrangement. In crystals, there is a close-range order as well as a long-range order and crystallization is primarily due to the distant arrangement. Under thermodynamic conditions where the crystalline state exists, only amorphous structures with a close order can be considered as instantaneous frozen states of liquids. This is the basis of the quasi-crystalline model of liquids and that is first given by Y.I. Frenkel. In this model, it is assumed that the motion of each liquid molecule from its oscillating motion in a crystalline-like close-order cell and this cell consists entirely of a certain free-leap in the order of transmission. The oscillation of the molecule in the cell is in complex nature. However, at the first approach, it can be assumed that this oscillation movement is harmonic. Then we can take the liquid as a set of harmonic oscillators. The latter is usually called **the harmonic oscillator model of the fluid**. Studies show that in many cases this model accurately describes the experimental results.

The first chapter concludes with an analysis of several approaches to surface tension of liquids. It is shown that historically, different approaches and models have been used to explain the phenomenon of surface tension in liquids and other related events.

The second chapter describes a new phenomenological method proposed by us for the first time and tested for surface

tension of a number of metallic and non-metallic fluids. This chapter also examines the relationship between surface tension and heat of surface formation. Using thermodynamic and potential methods, it was shown that the temperature dependence of the coefficient of surface tension in general

$$\frac{d\sigma}{dT} = -\frac{q}{T} \quad (2.1)$$

is given by the expression (q is the specific heat of surface formation).

Since the temperature dependence of the heat of surface formation is not taken into account and the critical temperature is $\sigma = 0$ then from (2.1)

$$\sigma = q \ln\left(\frac{T_c}{T}\right) \quad (2.2)$$

Becomes. On the other hand, $\ln\left(\frac{T_c}{T}\right) \approx 2\left(\frac{T_c-T}{T_c+T}\right)$ considering that from (2.2)

$$\sigma \approx 2q\left(\frac{T_c-T}{T_c+T}\right) \quad (2.3)$$

we get. (2.2), including (2.3) from a phenomenological point of view, in the case of heat of surface formation is not dependent on temperature then this is a general expression for the surface tension of liquids. Since the temperature of the crisis depends on the individuality of the fluid, it is natural that the surface tension must also be different for different fluids under the same physical conditions. Currently, almost since the critical temperature is known for all fluids, and the value of the surface tension coefficient at any temperature is known, it is possible to calculate the specific heat of surface formation from (2.2) or (2.3) and, as a result, to determine the analytical expression of the temperature dependence of surface tension. Of course, the latter is true only if the heat of surface formation does not depend on temperature. In this case, according to (2.3) $\sigma = f\left(\frac{T_c-T}{T_c+T}\right)$ a straight line must be observed in the coordinate system. The angle coefficient of this straight line will be two times the specific heat of surface formation temperature. The angle coefficient of this straight line will be twice the specific surface formation temperature. Based on the values of surface tension and

crisis temperature taken from the literature, appropriate calculations were performed for liquid alkali metals Na, K, Rb and Cs, and the calculated values for the temperature range 300-900 K are given in Table 2.1.

As can be seen there is no straight line that we recall for any of the taken liquids. This shows that the above hypothesis about the temperature dependence of the specific heat of surface formation is incorrect. As the temperature increases, the angle coefficient ($2q$) increases, and this increase is on average $\sim 10\%$ in the temperature range (400-900) K. The study of the possible temperature dependence of the specific heat of surface formation temperature shows that

$$q(T) = q_m - \alpha(T_m + T). \quad (2.4)$$

q_m the specific heat of the surface formation at the melting temperature, α - thermal coefficient, T_m -melting temperature of taken metal.

Table 2.1.
Verification of (2.3) for alkali metal liquids

T,K	$(T_c - T)/(T_c + T)$				$\frac{\sigma}{\left(\frac{T_c-T}{T_c+T}\right)} * 10, \text{erq/sm}^2$			
	Na	K	Rb	Cs	Na	K	Rb	Cs
350	-	0,7308	0,7143	0,7083	-	15,49	12,65	9,77
400	0,7241	0,6981	0,6800	0,6735	26,53	15,78	12,87	9,90
450	0,6949	0,6667	0,6471	0,6400	26,92	16,08	13,06	10,05
500	0,6667	0,6364	0,6154	0,6078	27,31	16,37	13,26	10,18
550	0,6393	0,6071	0,5849	0,5796	27,70	16,67	13,44	10,31
600	0,6192	0,5789	0,5556	0,5472	28,08	16,96	13,61	10,43
650	0,5873	0,5517	0,5273	0,5185	28,45	17,26	13,79	10,55
700	0,5625	0,5254	0,5000	0,4909	28,82	17,55	13,96	10,65
750	0,5384	0,5000	0,4737	0,4643	29,18	17,84	14,10	10,75
800	0,5151	0,4754	0,4483	0,4386	29,53	18,13	14,25	10,83
850	0,4925	0,4516	-	0,4138	29,87	18,42	-	19,90
900	0,4706	0,4286	0,400	0,3898	30,17	18,71	14,50	-

If the values of the surface tension coefficient T_i and T_j at two arbitrary temperatures σ_i and σ_j are known, taking into account that α does not depend on temperature,

$$\sigma(T) = [2q_m + \alpha(T_c + T - 2T_m)] \left(\frac{T_c - T}{T_c + T} \right) \quad (2.5)$$

we get.

For alkali metals $a \sim 10^2 \text{ erq/sm}^2$. According to (2.5), the surface tension coefficient of liquids should decrease with increasing temperature and should be zero at crisis temperature ($T = T_c$). Experience shows that the so-called regularities are actually observed.

The dependences (2.5) and (2.4) obtained for surface tension and heat of surface formation have been extensively studied and shown in the example of alkali metal fluids Na, K, Rb and Cs.

$$\alpha = \frac{1}{T_i - T_j} \left[\sigma_i \frac{T_b + T_i}{T_b - T_i} - \sigma_j \frac{T_b + T_j}{T_b - T_j} \right] \quad (2.6)$$

$$q_\sigma = \frac{1}{2} \left[\sigma \frac{T_b + T}{T_b - T} - \alpha(T_b + T - 2T_\sigma) \right] \quad (2.7)$$

Note that the calculation of α and q_m with the help of (2.6) and (2.7) allows us to determine the dependence of the surface tension coefficient $q = q(T)$ along with the temperature dependence.

Table 2.2
Quantities characterizing the heat of surface formation for alkali metal liquids

Matter	T_c, K	T_m, K	q_m, erq/sm^2	α, 10^2 $\frac{\text{erq}}{\text{sm}^2} \cdot \text{K}$
Na	2500	371	59,56	6,77
K	2250	337	20,0	5,90
Rb	2100	313	26,43	4,04
Cs	2050	302	28,10	2,35

The calculated values of α and q_m for alkali metal fluids, as well as

crisis (T_c) and melting (corresponding solid phase) (T_m) temperatures, are given in Table 2.2.

As can be seen from the table, it increases in α as the melting temperature increases. In terms of quality, this regularity can be explained by the decrease in bond energy at this transition $\text{Na} \rightarrow \text{K} \rightarrow \text{Rb} \rightarrow \text{Cs}$.

From the above explanation, it can be concluded that to calculate the temperature dependence of the surface tension coefficient of any liquid and the heat of surface formation, it is sufficient to know the values of surface tension at any two temperatures. Using this method, we calculated the coefficient of surface tension of alkali metals Na, K, Rb and Cs in the liquid phase and the specific heat of surface formation. It was found that the proposed method allows us to calculate the surface tension with a sufficiently high accuracy of $\sim 5\%$ and determine its temperature dependence. Analytical expressions of the dependencies $\sigma = \sigma(T)$ and $q=q(T)$ for the alkali metal fluids we studied are given in Table 2.3.

Thus, it has been commented on in this chapter shows that the semi-phenomenological method given by us on the phenomena of surface tension and heat of surface formation in liquids accurately reflects the experimental results.

Table 2.3

Analytical expression of surface tension and heat of surface formation of liquid metals

Liquid	$q, \text{erg}/\text{sm}^2$	$\sigma, \text{erg}/\text{sm}^2$
Na	$34,425 + 6,77 \cdot 10^{-2} \cdot T$	$[238,19 + 6,77 \cdot 10^{-2}] \frac{2500 - T}{2500 + T}$
K	$0,817 + 5,9 \cdot 10^{-2} \cdot T$	$[134,30 + 5,90 \cdot 10^{-2}] \frac{2250 - T}{2250 + T}$
Rb	$13,785 + 4,04 \cdot 10^{-2} \cdot T$	$[112,41 + 4,04 \cdot 10^{-2}] \frac{2100 - T}{2100 + T}$
Cs	$21,00 + 2,35 \cdot 10^{-2} \cdot T$	$[90,18 + 2,35 \cdot 10^{-2}] \frac{2050 - T}{2050 + T}$

The third chapter is devoted to a comparative analysis of the viscosity and various mechanisms of liquid metals and the interpretation of the semi-phenomenological viscosity mechanism proposed by us for the first time. This mechanism, first proposed by Prof. E.A. Eyvazov, is essentially a matter of the viscosity of a liquid between layers within a layer with a thickness of nanometers ($\sim 10 \text{ \AA}$) consists of the transmission of impulses by means of phonons. According to this mechanism since the internal friction force generated directly from adjacent Newtonian fluid between adjacent layers is $F_f = \eta \left(\frac{dv}{dr}\right) dS$, the dynamic viscosity in the case of a stationary flow

$$\eta = F_f \left[\left(\frac{dv}{dr}\right) dS \right]^{-1} \quad (3.1)$$

As can be seen, dynamic viscosity is the frictional force acting on a unit surface taken perpendicular to the gradient in the field of a single velocity gradient. Since the laminar flow is $\left(\frac{dv}{dr}\right) = \text{const}$, by marking $\left(\frac{dv}{dr} \cdot dS\right)^{-1} = B$, from (3.1)

$$\eta = B \cdot F_s \quad (3.2)$$

we get. In the potential field force with energy $U(r) = - \int F(r) dr$ since it is related to, (3.2)

$$\eta = -B \cdot \frac{dU(r)}{dr} \quad (3.3)$$

(3.3) is a general expression of viscosity, when the interaction potential $U(r)$ between the liquid particles is known allows to determine the obvious analytical expression of viscosity. However, it is clear that the $U(r)$ potential depends on the type of fluid - primarily the nature of the particles that make it up, it is in principle incorrect to look for a uniform regularity that is equally applicable to all liquids.

Numerous studies have shown that when most solids melt, the intermolecular distance increases (8÷10)%, and the force of intermolecular interactions remains the same as in the case of solid aggregates. Therefore, the known $U(r)$ potential for the solid phase can also be applied to the corresponding fluids. By accepting the existence of a short-range order in liquids, in terms of the latter, the viscosity of the liquid can be investigated with the help of (3.3). Note

that, in this case, the transmission of momentum between directly adjacent layers of nanometer thickness by the oscillating movement of particles located in these layers, that is, it occurs through phonons.

The expression (3.2) obtained from the phenomenological approach can be applied to all Newtonian fluids in general. For liquid metals, let us determine the expression of the interlayer interaction force and, consequently, the viscosity. For this purpose, let us assume that the motion of free electrons in an electrostatic potential field in a liquid metal is similar to that in a solid phase

$$U(r) = \frac{A}{r} \cdot e^{-Br} \quad (3.4)$$

is characterized by pseudopotential. Here, A -is constant and $B = \lambda^{-1}$

- (λ -Debye radius) depending on the nature of the ion. In the Thomas-Fermi theory of free electrons in metal, the shielding radius λ_{T-F} is practically independent of temperature and is determined by the concentration of free electrons and the Fermi energy corresponding to 0 K of the metal. Considering (3.4) in (3.3)

$$\eta = \frac{A}{r^2} - D = \eta_I + \eta_{II} \quad (3.5)$$

we get. Therefore, the viscosity of a metallic liquid consists of two limits (accumulation). It can be assumed that the first, $\eta_I = \frac{A}{r^2}$, which is inversely proportional to the square of the distance from the positively charged ion, is the viscosity due to the gravitational force. The fact that the second limit $\eta_{II} = -D$ is negative and does not depend on the distance between the ions suggests that it is associated with a free electron gas. Since the coefficient of thermal expansion of liquids is practically the same as the coefficient of thermal expansion of the corresponding solid phase, it can be assumed that the temperature dependence of the interatomic distance in a liquid is given by a linear law, ie $r \sim T$ - (remember that the volume of metal increases only 2 ÷ 5%). Then from the temperature dependence of the viscosity of the liquid metal (3.5)

$$\eta(T) \approx \frac{A}{T^2} - D \quad (3.6)$$

they are. That we use (3.6) is a general expression of the viscosity of liquid metals in the phenomenological approach. As can be seen, in

this case, the viscosity consists of the sum of the limits related to the ion subsystem and decreasing with the quadratic regularity with increasing temperature, and the limits independent of the temperature, which is related to the electronic subsystem and must be universal.

If the quantities A and D in expression (3.6) are known, the value of viscosity at any temperature can be calculated and thus the obvious expression of the temperature dependence of viscosity can be determined. The dissertation shows that the electron viscosity

$$\eta_e \approx \frac{2}{5e^2} m_e^* E_F \cdot \sigma^* \quad (3.7)$$

Here, σ^* -special electrical conductivity, E_F -Fermian energy and m_e^* -effective mass of electrons.

If we consider that, $E_F = \frac{\hbar^2}{2m_e} (3\pi^2 n_e)^{\frac{2}{3}}$ -then from (3.7)

$$\eta_e \approx \frac{1}{5} \left(\frac{\hbar^2}{e} \right) (3\pi^2 n_e)^{\frac{2}{3}} \cdot \sigma^* \quad (3.8)$$

we get. As can be seen, the electron viscosity in a liquid metal is determined by the concentration of free electrons and the specific electrical conductivity of the liquid. Since the concentration of free electrons does not depend on temperature and since the specific electrical conductivity decreases slightly with increasing temperature, the electron viscosity should decrease at first glance with increasing temperature. However, since the electrical conductivity of metals (in the liquid and solid phases) remains virtually constant at all temperatures, with the exception of the temperature region $T \leq 30 K$, it is natural that the electronic viscosity of the liquid metal will not change with temperature.

The calculated values of η_e of alkali liquid metals are given in Table 3.1. As can be seen from Table 3.1, the electron viscosity (η_e) is a significant part (~ 10%) of the total dynamic viscosity (η) of the liquid metal.

Thus, we can say that the dynamic viscosity of a liquid metal can be taken as the sum of the viscosities of ionic and free electron subsystems. The electron viscosity is about ~ 10% of the total viscosity and is determined only by Fermi energy and specific electrical resistance, regardless of temperature.

Table 3.1

Electronic viscosity of alkali metal liquids and a number of characteristic quantities.

Metal	E_F, eV	$n_e \cdot 10^{22}$	$\rho_{liq} \cdot 10^6$ <i>Om·sm</i>	$\eta \cdot 10^3$ <i>Pa·S</i>	$\eta_e \cdot 10^4$ <i>Pa·S</i>	$\lambda_{T-F} \cdot 10^9$ <i>sm</i>
Li	4,72	4,70	24,17	1,98	2,95	6,23
Na	3,23	2,65	9,6	4,79	3,96	6,68
K	2,12	1,40	13	6,33	3,71	7,43
Rb	1,85	1,15	22,5	6,60	1,87	7,68
Cs	1,58	0,91	37	8,54	0,97	7,99

It has been determined that for non-alkaline metal liquids, the same can be said about the viscosity (Table 3.2, Figure 3.1).

Table 3.2

$\eta = \eta(T)$ – analytical expression for non-alkaline metal liquids
(Viscosity is taken with $\frac{kq}{m \cdot san}$ – and T with K)

Liquid metal	Analitic expression of viscosity	Temperatur range
Pb	$\eta = \frac{621}{T^2} - 6,38 \cdot 10^{-4}$	$720 \leq T \leq 1100$
Sn	$\eta = \frac{363}{T^2} - 5,60 \cdot 10^{-4}$	$510 \leq T \leq 1100$
Zn	$\eta = \frac{1500}{T^2} - 2,75 \cdot 10^{-4}$	$720 \leq T \leq 970$
Hg	$\eta = \frac{70}{T^2} - 7,42 \cdot 10^{-4}$	$253 \leq T \leq 573$

Liquid metal can be considered as a solution consisting of a mixture of liquids that are physically compatible with the ionic and electron subsystems; each of the components of the solution to the physical properties of the liquid metal must give its supplement; In terms of application to dynamic viscosity, viscosity is equal to the

sum of ion (η_i) and electron (η_e) sums. Given the above, we can schematically show the temperature dependence of the dynamic viscosity of liquid metals as shown in Figure 3.2.

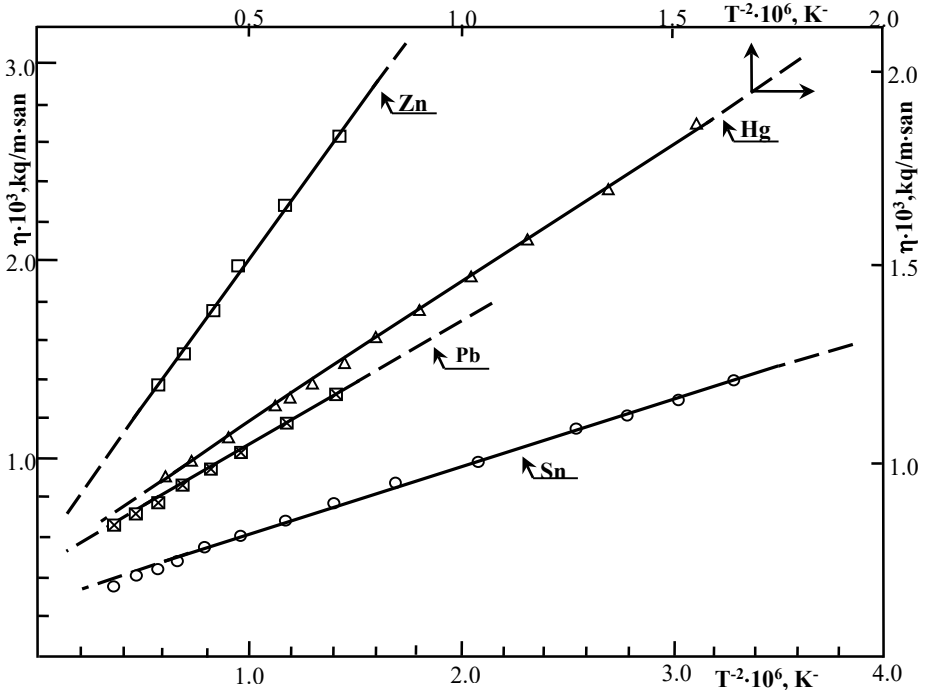


Figure 3.1. Temperature dependence of dynamic viscosity of non-alkali metals

Table 3.3

Temperature (T^*) and melting point (T_m) corresponding to the equality of the viscosity of the ion (η_i) and electron (η_e)

T, K	Liquid metals								
	Li	Na	K	Rb	Cs	Zn	Pb	Sn	Hg
T^*, K	808	917	797	742	701	2337	986	805	307
T_m, K	453,9	371,2	345,2	313,1	302,16	693,47	601,22	506,29	234,35
T^*/T_m	1,78	2,47	2,31	2,37	2,32	3,37	1,64	1,59	1,31

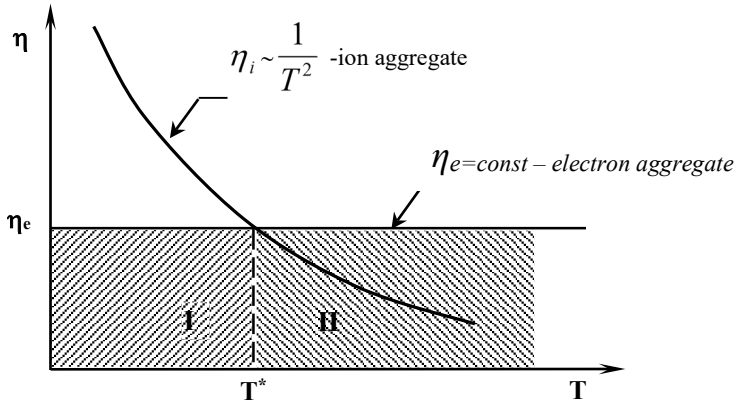


Figure 3.2. Schematic description of ionic (η_i) and electron (η_e) viscosities in liquid metals

For a number of liquid metals, the analytical expression for viscosity was determined using expression (3.6), and quantities A and D were estimated (Table 3.4).

Table 3.4
Calculated values of quantities A and D.

Liquid metal	A, $\frac{K^2 \cdot kq}{m \cdot san}$	D · 10⁶, $\frac{kq}{m \cdot san}$	Temp. range $\Delta T, K$
Li	95,84	-146,8	$500 \leq T \leq 1500$
Na	81,69	-97,1	$400 \leq T \leq 1500$
K	52,7	-83	$400 \leq T \leq 1500$
Pb	621	-638	$720 \leq T \leq 1100$
Sn	363	-560	$510 \leq T \leq 1100$
Hg	70	-242	$253 \leq T \leq 573$

As can be seen from Table (3.4), in liquids of metals having a similar (same type) crystal lattice in the solid phase, the quantities A and D decrease in the corresponding transitions (Li → Na →

K and Pb → Sn → Hg). Most likely, this is due to the electronic structure of metals. The calculated and table values of viscosity at temperatures above boiling point differ slightly. It can be assumed that harmonic convergence at high temperatures does not justify itself and it is not correct to take the potential of intermolecular interactions in the form of pseudopotential.

The fourth chapter is devoted to the study of the correlation between the volume and surface properties of metallic fluids. The possibility of this correlation is primarily due to the fact that the force of interaction between particles (atoms or molecules) located on the surface and in volume is of the same nature. The probability of this correlation is primarily due to the fact that the interaction force between particles (atoms or molecules) on the surface and volume is of the same quality. In Chapters II and III of the dissertation it is established that viscosity and surface tension in liquid metals are nano-phenomena related to the movement and interaction of liquid molecules located in the nanometer-order surface layer. Therefore, in terms of general physical principles, a correlation can be expected between them. Paragraph 3 of Chapter 4 is devoted to the study of the possible relationship between surface tension and viscosity in the example of liquid alkali metals. It was determined that the viscosity (η_f) of liquid alkali metals, which we calculated phenomenologically, is related to the coefficient of surface tension at the appropriate temperature. The $\eta = f(\sigma)$ dependence for a number of metal fluids is given in Figure 4.1. For all three fluids, this dependence is the same: with a decrease in surface tension, the viscosity decreases sharply (at low temperatures): but at high temperatures the rate of reduction slows down and finally approaches a constant value. In this dissertation it was shown that this dependence

$$\eta_{\sigma}(T) = \eta_0 + A \left(\frac{T_b - T}{T} \right) \cdot \sigma \quad (4.1)$$

is given by the analytical expression. In (4.1) η and at $\sigma - T$ temperatures, respectively viscosity and surface tension, T_c – critical temperature, η_0 – viscosity at critical temperature, A – correlation coefficient.

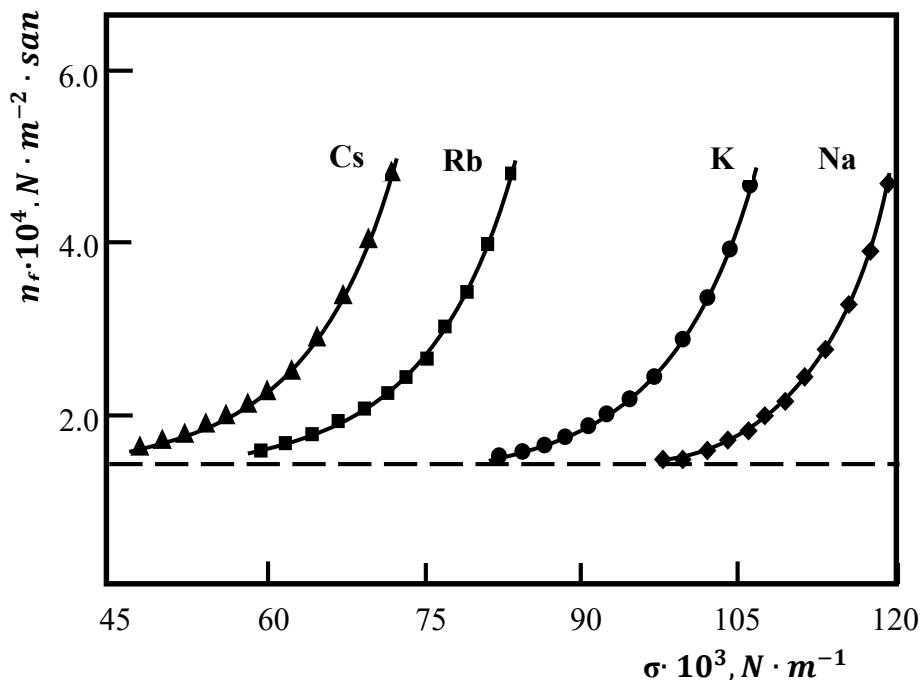


Fig.4.3. Dependence of viscosity on surface tension

$$\eta_{\sigma}(T) = \eta_0 + A \left(\frac{T_b - T}{T} \right) \cdot \sigma \quad (4.1)$$

is given by the analytical expression. In (4.1) η and at $\sigma - T$ temperatures, respectively viscosity and surface tension, T_c – critical temperature, η_0 – viscosity at critical temperature, A – correlation coefficient.

Note that, (4.1) is an analytical expression that reflects the dependence of the dynamic viscosity of alkali metal fluids on the coefficient of surface tension over a wide temperature range up to the critical temperature.

Obviously, if the quantities A and η_0 are known, $\eta = \eta(\sigma)$ – can be written explicitly with the help of (4.1): Knowing the values

of η and σ at two arbitrary T_i and T_K temperatures with the help of (4.1)

$$A = \Delta\eta_{ik} \left[\left(\frac{\sigma_i}{T_i} - \frac{\sigma_K}{T_K} \right) \cdot T_b - \Delta\sigma_{ik} \right]^{-1} \quad (4.2)$$

we get. Considering (4.2) in (4.1), we can determine η_0 .

The viscosity values calculated according to the interpreted procedure (4.1) correspond to the phenomenologically calculated value with sufficient accuracy ($\sim <15\%$), which indicates the suitability of the analytical expression (4.1) we defined for alkali metal liquids. We have shown that it is $A = \xi \cdot \left(\frac{\mu}{N_A \cdot E_r} \right)^{\frac{1}{2}}$ (μ -molecular weight, N_A -Avogadro's number, E_b -bond energy, ξ - dimensionless constant). Considering the latter, from (4.1)

$$\eta_\sigma = \eta_0 + \xi \cdot \left(\frac{\mu}{N_A \cdot E_r} \right)^{\frac{1}{2}} \cdot \frac{T_b - T}{T} \cdot \sigma \quad (4.3)$$

they are. (4.3) relates the viscosity and the surface tension coefficient by means of parameters that characterize the liquid from a microscopic point of view. If other quantities included in this expression are known, the bond energy can be estimated.

Results

1. It was determined by examining the relevant literature that the surface tension and dynamic viscosity of liquids are related to the presence of a subsurface layer, which is determined by the intermolecular interactions that occur in this physical layer. Since the thickness of the physical layer is in the order of nanometers, both events studied can be considered as a special case of a general nanophenomena;

2. Using the methods of thermodynamics and pseudo-potentials, new analytical regularities have been identified that describe the surface tension and dynamic viscosity over a wide temperature range. Until then, the calculated values of viscosity and surface tension of liquid metals are consistent with the table values with an error of $\lesssim 10\%$. It is shown that the proposed method does

not depend on the individuality of the liquid and is universal for liquid metals;

3. It has been determined that the hydrodynamic model cannot be applied to alkali metal fluids and for these fluids, the Stokes-Einstein accordance is useless, that is self-diffusion and dynamic viscosity occur by different mechanisms - due to diffusion density fluctuations, and viscosity occurs under the influence of the force field;

4. It was found that the liquid metal is a unique binary solution: It is a system formed by free electrons and ions. The viscosity of a liquid metal consists of the sum of ions and electrons. A method has been developed to determine the (η_i) ion and (η_e) electron accumulations of viscosity, and it has been shown in the example of alkali metal liquids that $\eta_i \approx 10\eta_e$, $\eta_i \sim T^{-2}$ and $\eta_e = \text{const}$;

5. It is concluded that dynamic viscosity is a non-activating process up to high temperatures not very close to the boiling point, which occurs due to the transfer of phonons and the kinetic movement of free electrons inside the nano layer;

6. For the first time, a correlation between the dynamic viscosity of liquid metals and the coefficient of surface tension was determined and it was shown that based on this correlation it is possible to estimate the intermolecular bond in liquids;

7. The present dissertation provides a basis for classifying surface tension and dynamic viscosity not as a phenomenon of molecular transfer occurring in a macroscopic volume, but as a nano phenomenon established in a subsurface layer of several angstroms;

8. Correlation between the coefficient of surface tension and the coefficients of thermal contraction and expansion was determined and based on this, the thickness of the subsurface layer was estimated.

The main part of the dissertation is published in the following works

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The defense of the dissertation will be held on 08 April 2022 at 15⁰⁰ in the meeting of the Dissertation Council ED 2.19 operating under Baku State University.

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The dissertation is accessible at the Scientific Library of Baku State University.

Electronic versions of dissertation and its abstract are available on the official website of Baku State University.

Abstract was sent to the required addresses on 05 March in 2022.

Signed for print: 28.02.2022

Paper format: A5

Volume: 25751

Number of hard copies: 100