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EVIDENCE OF THE COLLECTIVE TRANSPORT IN ATOMIC LIQUIDS AND LIQUID METALS

The behavior of the effective radii of "particles" (molecules and ions) as a manifestation of the collective components of their thermal motion in atomic liquids and liquid metals has been studied. The specific form of the temperature dependence of the effective radii of molecules and ions is established in good agreement with the results obtained for the hydrodynamic radii according to the Stokes–Einstein formula. Attention is drawn to the differences between the values of the radii of particles that are used to describe the thermodynamic and kinetic properties of liquids.

Keywords: thermal motion of molecules, collective transport, self-diffusion coefficient of molecules in liquids.

1. Introduction

The existence of a collective transport in liquid water was predicted in work [1]. The extended theory of collective mass transfer was initiated by I.Z. Fisher in work [2]. The works [3–6] were devoted to the further development and improvement of theoretical ideas about the nature of collective transport. An extremely important role in the formation of ideas concerning the collective transport in liquids was played by the works of Bulavin *et al.* [7–11]. In those works, as well as in the works by Mykhailenko and *et al.* [12, 13] dealing with computer simulations, it was proved that the collective component in the self-diffusion coefficient can reach a quarter of its total magnitude.

However, no complete agreement between theoretical and experimental data has been attained, because the so-called "single-particle" component (see works [2, 14]) of the self-diffusion coefficient remained unknown. Moreover, it was assumed that the temperature dependence of this component may have an activation character, similar to what takes place in solids. The falsity of such ideas has been emphasized many times in works [6, 14–19]. In works [6, 16, 18], it was ultimately proved that the so-called "single-particle" component of the self-diffusion coefficient emerges owing to the swings of small molecular groups at small angles. A typical molecular group of this kind is formed by a certain molecule and its immediate molecular environment. Of course, the group swing motions have no activation character, but a collective one.

As was shown in work [16], the "single-particle" component is described by the Stokes–Einstein formula in which the radius of the molecule is determined from the analysis of the shear viscosity. As a result, the self-diffusion coefficient of a molecule is expressed by the sum (see also works [14, 17])

$$D_s = D_r + D_c, \tag{1}$$

where

$$D_c = \frac{k_\mathrm{B} T}{10\pi\eta\sqrt{\nu\tau_\mathrm{M}}} \tag{2}$$

is a collective component associated with the nanoscopic hydrodynamic vortex modes, and

$$D_r = \frac{k_\mathrm{B} T}{6\pi\eta r_p^{(\nu)}} \tag{3}$$

is a contribution from the swing motions of small molecular groups. Here, k_B is the Boltzmann constant, T the temperature, η the dynamic shear viscosity, ν the kinematic shear viscosity, and τ_M the Maxwell relaxation time.

Table 1. **Values of the parameters in formula (1)**

Parameter	Ar	Ne	Kr	Xe	C_6H_6	N_2	Sn	Bi	Pb
$\tilde{v}_0$	0.984	0.978	0.985	0.982	0.976	0.977	0.993	0.960	0.981
ζ_0	0.263	0.278	0.264	0.296	0.285	0.294	0.211	0.342	0.310
$(1-\tilde{v}_0)^{1/3}$	0.251	0.279	0.243	0.261	0.288	0.284	0.190	0.342	0.272

Writing the molecular self-diffusion coefficient in the form

$$D_s(T)=\frac{k_BT}{6\pi\eta r_p^{(D)}},$$

we obtain the following formula for the hydrodynamic radius of a molecule:

$$r_P^{(D)}(T)=\frac{k_BT}{6\pi\eta D_s(T)}. \qquad (4)$$

The temperature dependence $r_P^{(D)}(T)$ was the subject of research in a lot of works [19–22]. First of all, this concerns liquid metals, where $r_P^{(D)}$ has to be identified with the ionic radius, $r_I(T)=r_P^{(D)}(T)$. However, there are a lot of misunderstandings about the temperature dependence of r_I.

In the framework of our approach, the corresponding radius of a particle, which will be called its effective radius, is determined by the relations

$$\frac{1}{r_p^{(\text{eff})}(T)}=\frac{1}{r_p^{(\nu)}}+\frac{3}{5\sqrt{\nu(T)\tau_{\text{M}}(T)}}, \qquad (5)$$

where $r_P^{(\text{eff})}(T)$ is a known temperature dependence. In this work, the temperature dependences of the radii $r_p^{(\text{eff})}$ and $r_p^{(D)}$ will be studied in detail for argon-like liquids and liquid metals. Under argon-like liquids, we understand all low-molecular liquids for which the averaged potentials of intermolecular interaction possess the argon-like structure. This class of liquids includes argon and other atomic liquids according to Bulavin's classification [23], liquids with dumbbell-like molecules of the N_2 type and disc-like molecules of the C_6H_6 type, and some other liquids. A good numerical agreement between the values of $r_p^{(\text{eff})}(T)$ and $r_p^{(D)}(T)$ is considered as a clear criterion for the existence of the collective transport in liquids. A direct equivalent of this criterion is the agreement between the experimental values of the self-diffusion coefficient and the values calculated by formula (1).

2. Shear Viscosity in Argon-Like Liquids and the Determination of the Molecular and Ionic Radii

As was shown in works [24–27], the kinematic shear viscosity of liquids is mainly determined by the effects of friction between molecular layers that move relative to one another. This parameter is described by the equation

$$\tilde{\nu}(\tilde{v},t)\approx\left[\frac{1-\tilde{v}_0^{(i)}}{\tilde{v}-\tilde{v}_0^{(i)}(t)}\right]^{1/3} \qquad (6)$$

for $i=$ Ar, Kr, C_6H_6, $C_6H_5NO_2$, N_2, and so forth, where $\tilde{\nu}(t)=\nu(t)/\nu_{\text{tr}}$; ν_{tr} is the kinematic shear viscosity at the triple point, $t=T/T_{\text{tr}}$ and $\tilde{v}=v/v_{\text{tr}}$ are the dimensionless temperature and specific volume, respectively (T_{tr} and v_{tr} are the temperature and the specific volume, respectively, at the triple point); $\tilde{v}_0^{(i)}=v_0^{(i)}/v_{\text{tr}}^{(i)}$, and $v_0^{(i)}$ is the excluded volume of the system, which corresponds to its shear viscosity. Formula (6) successfully describes the shear viscosity in all liquids for which the averaged intermolecular potentials are similar to the Lennard-Jones potential in argon. It reproduces the temperature dependence of the shear viscosity with a high accuracy in such liquids as benzene, nitrobenzene, and nitrogen [25], as well as in liquid alkali [28] and transition metals [29].

Table 1 contains the values of the parameters entering formula (6) for various liquids. As one can see, the values of the excluded volume $\tilde{v}_0$ are almost identical to the values of the specific volume in the indicated liquids at the corresponding triple point. Such a situation also takes place for alkali and post-transition metals. In the following calculations, we will assume that $v_0\approx v_m$.

In work [25], it was shown that formula (6) also well reproduces the shear viscosity of water almost within the entire temperature interval of its liquid state: 315 K $< T <$ 620 K. We emphasize once more that the values of the excluded volume almost coincide with the values of the specific volume at the triple point for liquids or the melting point for metals. This fact is another confirmation that there is no activation mechanism of the shear viscosity and self-diffusion processes in liquids.

The analysis of the kinematic shear viscosity makes it possible to determine the radii $r_p^{(\nu)}$ of molecules or ions in liquid metals. As it is in the van der Waals equation, the excluded volume of a particle is equal to four times its proper volume. Therefore, the particle radius $r_p^{(\nu)}$ can be calculated using the formula

$$r_p^{(\nu)} = \left(\frac{3}{16\pi} v_m\right)^{1/3}.$$

In liquid metals, an important role is played by the parameter of dense packing of ions, δ, which is defined as the ratio between the intrinsic volume of the ion and the volume per ion in the system, i.e. as the ratio between the intrinsic volume of the ion and the volume of the sphere whose radius coincides with the position of the maximum in the binary correlation function for the system of solid spheres [30, 31]. For alkali metals, this parameter takes the values $\delta = 0.46 \div 0.48$ [32]. Therefore, the ionic radius turns out related to the specific volume as follows:

$$r_p^{(\nu)} = \left(\frac{3}{16\pi} \delta \nu_m\right)^{1/3}.$$

The values of the radii $r_p^{(\nu)}$ of molecules and ions together with the corresponding values for the gas phase of the corresponding liquid, $r_p^{(\mathrm{gas})}$, and the values used in the Lennard-Jones potentials, $r_p^{(\mathrm{LJ})}$, are quoted in Tables 2 and 3, respectively. As one can see, the molecular radii determined from the equation of state and from the analysis of the kinematic shear viscosity are appreciably different from each other (e.g., $r_p^{(\mathrm{LJ})}/r_p^{(\nu)} \approx 1.21$ for argon). A similar situation is also typical of the radii $r_p^{(\nu)}$, which are determined from the shear viscosity of gases [33], but the corresponding difference between $r_p^{(\mathrm{LJ})}$ and $r_p^{(\nu)}$ is smaller.

Let us illustrate the origin of this situation by estimating the radius that is responsible for the values of thermodynamic quantities and the radius that determines the kinetic characteristics. The former roughly corresponds to the position of the minimum in the intermolecular potential, $U'(r_p) = 0$, whereas the latter is determined by the value of the potential core radius at which $U(r_p) \approx k_\mathrm{B} T_\mathrm{tr}$. In the case of argon, the ratio between those two radii $r_p^{(\mathrm{LJ})}/r_p^{(\nu)} \approx 1.16$.

The ionic radii in liquid metals, which are determined from the equation of state and by analyzing the kinematic shear viscosity, differ from each other, as it is for molecular liquids, but the difference is somewhat larger. This situation arises due to a "softer" repulsion between the ions. It can be demonstrated using the general view of the potential from works [36, 37]. In particular, the ratio $r_p^{(\mathrm{LJ})}/r_p^{(\nu)}$ between those two radii is approximately equal to 1.2 for liquid Na, and 1.29 for liquid Rb, which approximately corresponds to the ratio of radii taken from Table 3 [28].

3. Estimation of the Maxwell Relaxation Time in Liquids and Liquid Metals and Its Temperature Dependence

By definition, the Maxwell relaxation time (MRT) equals [38, 39]

$$\tau_\mathrm{M} = \eta / G, \tag{7}$$

where η is the dynamic shear viscosity in a liquid, and G the high-frequency shear modulus in the liquid

Table 2. **Molecular radii (in Å units) obtained from the equation of state, $r_p^{(\mathrm{LJ})}$, and by analyzing the kinematic shear viscosity, $r_p^{(v)}$**

Radii of molecules	Ar	Kr	C_6H_6	$C_6H_5NO_2$	N_2
$r_p^{(v)}$	1.411	1.55	2.19	2.38	1.49
$r_p^{(\mathrm{LJ})}$	1.701	1.77	2.62	2.80	1.85
$r_p^{(\mathrm{gas})}$	1.73	1.80	2.63	–	1.82

Table 3. **Ionic radii (in Å units) obtained from the equation of state, $r_p^{(\mathrm{LJ})}$, and by analyzing the kinematic shear viscosity, $r_p^{(v)}$**

Radii of molecules	Li^+	Na^+	K^+	Rb^+	Pb^+	Sn^+	Bi^+
$r_p^{(v)}$	0.79	1.01	1.23	1.52	1.18	1.24	1.27
$r_p^{(\mathrm{LJ})}$	1.27 [34]	1.13 [34]	1.62 [35]	2.02 [20]	1.7 [34]	–	–

Table 4. **The upper limits T_u of the temperature interval $T_m < T < T_u$, where the calculated MRT has physically correct values**

	Ar	Kr	C_6H_6	$C_6H_5NO_2$	N_2	Na^+
T_u	$1.19T_m \approx 100$ K	$1.14T_m \approx 132$ K	$1.42T_m \approx 400$ K	$1.33T_m \approx 375$ K	$1.31T_m \approx 83$ K	$1.10T_m \approx 1132$ K

system. Making use of the kinematic shear viscosity $\nu = \eta/\rho$ and the relationship $G = \rho c_t^2$, we obtain

$$\tau_\mathrm{M} = \nu/c_t^2,$$

where

$$\tau_\mathrm{M} = \nu/c_t^2$$

is the high-frequency velocity of transverse sound in liquids. Taking the inequality $c_t < c_l$ into account, we obtain

$$\tau_\mathrm{M} > \nu/c_l^2 \tag{8}$$

for the lower MRT limit. Making allowance for the approximate relationship $c_t^2 \approx \frac{2}{3}c_l^2$ between the velocities of transverse and longitudinal sounds [40, 41], we get

$$\tau_\mathrm{M} = \frac{3\nu}{2c_l^2}.$$

For atomic and low-molecular liquids, the temperature dependence of the longitudinal sound velocity is known, so the fulfillment of inequality (8) is mandatory. For liquid metals, the temperature dependence of the longitudinal sound velocity has not been studied so well, so Eq. (7) was used to calculate τ_M with an acceptable accuracy. In the latter case, the MRT equals

$$\tau_\mathrm{M}(T) = \tau_\mathrm{M}(T_m)\frac{\eta(T)}{\eta(T_m)}, \tag{9}$$

where

$$\tau_\mathrm{M}(T_m) = \frac{\eta(T_m)}{G_\mathrm{cr}}$$

is the MRT value at the melting point. The scope of MRT applications is limited from above by the temperature T_u determined from the equation

$$\frac{\nu(T_u)}{c_l(T_u)} = \sqrt{\frac{3}{2}}\,r_p. \tag{10}$$

Here, the argument was used that the radius of the Lagrangian particle, $r_L = 2\sqrt{\nu\tau_\mathrm{M}}$ has to be not smaller than the radius of the molecular complex consisting of the selected molecule and its immediate environment. The values of the temperatureT_u are quoted in Table 4.

4. Comparison of the $r_p^{(\mathrm{eff})}(T)$- and $r_p^{(D)}(T)$-Values for Lliquids and Liquid Metals

Let us compare the values of the effective and hydrodynamic molecular (ionic) radii making use of formulas (4) and (5). In Fig. 1, the temperature dependences of those parameters are illustrated for some liquids.

For all liquids, the effective and hydrodynamic radii of particles demonstrate a similar temperature behavior. Taking the collective contribution to the self-diffusion coefficient of particles in liquids into account exhaustively explains the necessity of the artificial introduction of the particle radius dependence on the temperature when comparing the theoretical and experimental values of $D_s(T)$ on the basis of the Stokes–Einstein formula. However, the $r_p^{(\mathrm{eff})}$- and $r_p^{(D)}$-values also reveal some difference. First of all, this is a result of the measurement accuracy of self-diffusion coefficients, which amounted to about 10% or less in most experiments. Approximately the same discrepancy takes place between the $r_p^{(\mathrm{eff})}$- and $r_p^{(D)}$-values. For liquid Na and Pb, the measurement accuracy of the corresponding self-diffusion coefficients was about 6%. So, as one can see, the $r_p^{(\mathrm{eff})}$- and $r_p^{(D)}$-values are practically identical, within the measurement error for $D_s(T)$ in the temperature interval, where the collective motion of particles must be taken into account.

Another origin of the discrepancies between $r_p^{(\mathrm{eff})}$ and $r_p^{(D)}$ is the calculation error for the MRT parameter, which is determined by the transverse sound velocity. There are experiments, where the trans-

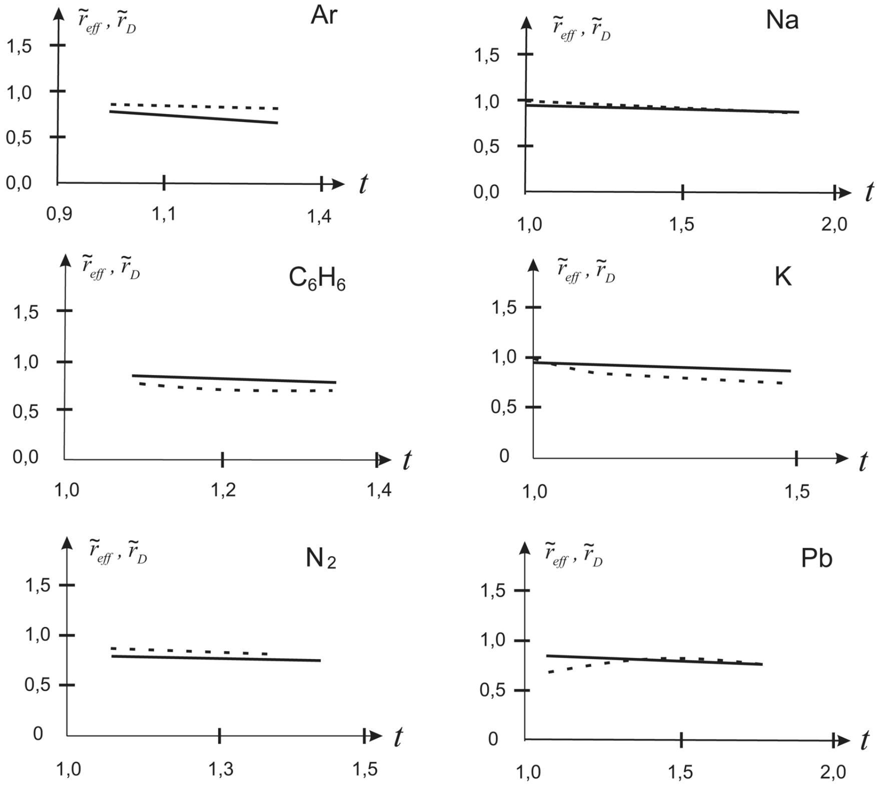

Fig. 1. Dependences of $\tilde{r}_{\text{eff}} = r_p^{(\text{eff})}/r_p^{(\nu)}$ (solid curves) and $\tilde{r}_D = r_p^{(D)}/r_p^{(\nu)}$ (dotted curves) on the normalized temperature T/T_{tr} (T/T_m for liquid metals) for argon-like liquids and liquid metals

verse sound velocity was measured for highly viscous liquids [42]. For atomic and low-molecular liquids, the MRT was calculated using molecular dynamics [6, 43, 44]. However, we do not know about such experiments or theoretical calculations for liquid metals. Nevertheless, despite the indicated uncertainties, the $r_p^{(\text{eff})}$-values practically coincide with the $r_p^{(D)}$-ones to the measurement error of the self-diffusion coefficient and correctly describe the temperature dependence of the hydrodynamic particle radius. Thus, taking the component D_c of the self-diffusion coefficient into account is crucial for a wide scope of liquids: atomic, low-molecular ones, and pure liquid metals.

5. Discussion of the Results Obtained

In this work, a clear definition of the effective radius $r_p^{(\text{eff})}$ of molecules and ions was given, and, on the basis of many liquids taken as examples, it was shown that $r_p^{(\text{eff})}(T) \approx r_p^{(D)}(T)$. This relationship is a strong evidence of the existence of a collective transport in liquids and liquid metals. It was shown above that the accuracy of this approximate equality depends, first of all, on the measurement accuracy of the self-diffusion coefficient values, as well as on the determination accuracy of the Maxwell relaxation time.

Let us discuss the comparison of our results with those obtained in works [20, 45] for alkali metals Rb and Cs in more detail. According to work [45], main attention at the first stage was paid to the calculation of the effective interaction potential between two ions. For this purpose, the cited authors used the Schommers algorithm [46]. Then, using the molecular dynamics method, the mean-square displacement of the ion, $\langle(\Delta\mathbf{r})^2\rangle$, was calculated and, with the help of the relation

$$D_s = \lim_{t\to\infty} \frac{\langle(\Delta\mathbf{r})^2\rangle}{6t},$$

the values of the ionic self-diffusion coefficient were determined. This circumstance is especially impor-

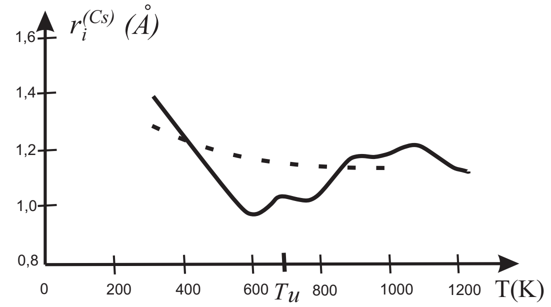

Fig. 2. Temperature dependences of $r_D^{(\mathrm{Cs})}$ (solid curve) and $r_{\mathrm{eff}}^{(\mathrm{Cs})}$ (dotted curve). The marker T_u denotes the upper limit of the temperature interval, where the MRT values for liquid Cs are physically correct

tant, because the experimental values of the self-diffusion coefficient D_s were obtained only for three temperatures: 301.8, 573, and 773 K. The $D_s^{(\mathrm{Cs})}$-values calculated in work [45] correspond to a rather wide temperature interval 306 K $< T <$ 1400 K, being in a quite satisfactory agreement with experimental data.

Below, we used the values D_s for Cs that were obtained in work [45]. The radius $r_D^{(\mathrm{Cs})}$ of a Cs$^+$ cation was determined with the help of the Stokes–Einstein relation $r_p^{-1} \sim D_s\eta/T$. The values of the radius $r_D^{(\mathrm{Cs})}$ obtained in this way and the radius $r_{\mathrm{eff}}^{(\mathrm{Cs})}$ calculated using formula (5) are compared in Fig. 2. When calculating $r_{\mathrm{eff}}^{(\mathrm{Cs})}$, the value $r_p^{(\mathrm{Cs})} = 1.495$ Å corresponding to the shear viscosity of the melt was used instead of $r_p^{(\mathrm{Cs})}$, and the MRT was calculated by formula (7). The temperature dependence of $r_{\mathrm{eff}}^{(\mathrm{Cs})}$ becomes appreciable only in the temperature interval 306 K $< T <$ 700 K, where the collective contribution to D_s has to be taken into account. In what follows, we took $r_{\mathrm{eff}}^{(\mathrm{Cs})} \to r_p^{(\mathrm{Cs})}$.

As one can see, the calculated ion radii agree with one another by the order of magnitude, but the temperature dependence of $r_D^{(\mathrm{Cs})}$ is substantially nonmonotonic, although there are no physical grounds for such nonmonotonic behavior. From the comparison made above, it follows that the temperature dependence of $r_{\mathrm{eff}}^{(\mathrm{ion})}$ is completely governed by the collective drift of a molecule or ion in the field of thermal hydrodynamic nanoscopic fluctuations.

In work [21], the temperature dependences of the self-diffusion coefficients of Al$^+$ and Ni$^+$ cations in Al–Ni melts were studied. It was shown that there are intervals, where the temperature dependences of $r_D^{(i)}$ ($i =$ Al$^+$ and Ni$^+$) are strong. Unfortunately, our results cannot yet be compared with the results of work [21] because of the lack of reliable values for the shear viscosity coefficient obtained at various temperature and melt concentration values.

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1. V.S. Oskotskii. To the theory of quasielastic scattering of cold neutrons in liquid. *Fiz. Tverd. Tela* **5**, 1082 (1963) (in Russian).
2. I.Z. Fisher. Hydrodynamic asymptotics of autocorrelation function of molecular velocity in classical fluid. *Zh. Eksp. Teor. Fiz.* **61**, 1647 (1971) (in Russian).
3. T.V. Lokotosh, N.P. Malomuzh. Lagrange theory of thermal hydrodynamic fluctuations and collective diffusion in liquids. *Physica A* **286**, 474 (2000).
4. L.A. Bulavin, T.V. Lokotosh, N.P. Malomuzh. Role of the collective self-diffusion in water and other liquids. *J. Mol. Liq.* **137**,1 (2008).
5. T.V. Lokotosh, N.P. Malomuzh, K.N. Pankratov. Thermal motion in water-electrolyte solutions according to quasielastic incoherent neutron scattering data. *J. Chem. Eng. Data* **55**, 2021 (2010).
6. T.V. Lokotosh, M.P. Malomuzh, K.M. Pankratov, K.S. Shakun. New results in the theory of collective self-diffusion in liquids. *Ukr. J. Phys.* **60**, 697 (2015).
7. L.A. Bulavin, P.G. Ivanitskii, V.G. Krotenko, V.N. Lyaskovskaya. Neutron studies of water self-diffusion in aqueous electrolyte solutions. *Zh. Fiz. Khim.* **61**, 3270 (1987) (in Russian).
8. L.A. Bulavin, A.A. Vasilkevich, A.K. Dorosh, V.T. Krotenko, V.I. Slisenko. Self-diffusion of water in aqueous solutions of singly charged electrolytes. *Ukr. Fiz. Zh.* **31**, 1703 (1986) (in Russian).
9. V.T. Krotenko, A.K. Dorosh, P.G. Ivanitskii, L.A. Bulavin, V.I. Slisenko, A.A. Vasilkevich. Neutron studies of self-diffusion of water molecules in electrolyte solutions. *Zh. Strukt. Khim.* **33**, 72 (1992) (in Russian).
10. L.A. Bulavin, N.P. Malomuzh, K.N. Pankratov. Self-diffusion features in water. *Zh. Strukt. Khim.* **47**, S54 (2006) (in Russian).
11. L.A. Bulavin, N.P. Malomuzh, K.N. Pankratov. The character of the thermal motion of water molecules according to the data of quasielastic incoherent scattering of slow neutrons. *Zh. Strukt. Khim.* **47**, 54 (2006) (in Russian).
12. S.A. Mikhailenko, V.V. Yakuba. Self-diffusion and nuclear magnetic relaxation in liquid mixtures CH_4-CF_4. *Ukr. Fiz. Zh.* **26**, 784 (1981) (in Russian).

13. S.A. Mikhailenko, V.V. Yakuba. Self-diffusion and nuclear magnetic relaxation in liquid propylene and its mixtures with krypton. *Ukr. Fiz. Zh.* **27**, 712 (1982) (in Russian).
14. N.P. Malomuzh, I.Z. Fisher. On the collective nature of thermal motion in liquids. *Fiz. Zhidk. Sost.* No. 1, 33 (1973) (in Russian).
15. I.V. Blazhnov, N.P. Malomuzh, S.V. Lishchuk. Temperature dependence of density, thermal expansion coefficient and shear viscosity of supercooled glycerol as a reflection of its structure. *J. Chem. Phys.* **121**, 6435 (2004).
16. N.P. Malomuzh, V.N. Makhlaichuk. Theory of self-diffusion in liquid metals. *Rasplavy* **5**, 561 (2018) (in Russian).
17. N.P. Malomuzh. Nature of self-diffusion in fluids. *Ukr. J. Phys.* **63**, 1076 (2018).
18. R.A. Swalin. On the theory of self-diffusion in liquid metals. *Acta Metallurgica* **7**, 736 (1959).
19. D.K. Belashchenko. Computer simulation of liquid metals. *Usp. Fiz. Nauk* **183**, 1281 (2013) (in Russian).
20. D.K. Belashchenko. Embedded atom model application to liquid metals: Liquid rubidium. *Russ. J. Phys. Chem.* **80**, 1567 (2006).
21. N. Jakse, A. Pasturel. Transport properties and Stokes–Einstein relation in Al-rich liquid alloys. *J. Chem. Phys.* **144**, 244502 (2016).
22. F. Demmel, A. Tani. Stokes–Einstein relation of the liquid metal rubidium and its relationship to changes in the microscopic dynamics with increasing temperature. *Phys. Rev. E* **97**, 062124 (2018).
23. L.A. Bulavin. *Neutron Diagnostics of Liquid Matter State* (Institute for Safety Problems of Nuclear Power Plants of the NAS of Ukraine, 2012) (in Ukrainian).
24. N.P. Malomuzh , V.P. Oleynik. Nature of the kinematic shear viscosity of water. *J. Struct. Chem. (Russia)* **49**, 1055 (2008).
25. P.V.Makhlaichuk, V.N.Makhlaichuk, N.P.Malomuzh. Nature of the kinematic shear viscosity of low-molecular liquids with averaged potential of Lennard-Jones type. *J. Mol. Liq.* **225**, 577 (2017).
26. L.A. Bulavin, A.I. Fisenko, N.P. Malomuzh. Surprising properties of the kinematic shear viscosity of water. *Chem. Phys. Lett.* **453**, 183 (2008).
27. V.M. Makhlaichuk. Qualitative properties of shear viscosity in liquids. *Ukr. J. Phys.* **63**, 986 (2018).
28. V.N. Makhlaichuk. Kinematic shear viscosity of liquid alkaline metals. *Ukr. J. Phys.* **62**, 672, (2017).
29. N.P. Malomuzh, V.N. Makhlaichuk. Peculiarities of self-diffusion and shear viscosity in transition and post-transition metals. *Rasplavy* **5**, 578 (2018) (in Russian).
30. N.W. Ashcroft, J. Lekner. Structure and resistivity of liquid metals. *Phys. Rev. B* **45**, 83 (1976).
31. D.K. Belashchenko. *Transfer Phenomena in Liquid Metals and Semiconductors* (Atomizdat, 1970) (in Russian).
32. P. Protopapas, H.C.Andersen, N.A.D. Parlee. Theory of transport in liquid metals. I. Calculation of self-diffusion coefficients. *J. Chem. Phys.* **59**, 15 (1973).
33. J.O. Hirschfelder, Ch.F. Curtiss, R.B. Bird. *Molecular Theory of Gases and Liquids* (Wiley, 1967).
34. H.M. Lu, G. Li, Y.F. Zhu, Q. Jiang. Temperature dependence of self-diffusion coefficient, *J. Non-Cryst. Solids* **352**, 2797 (2006).
35. S. Koneshan, J.C. Rasaiah, R.M. Lynden-Bell, S.H. Lee. Solvent structure, dynamics, and ion mobility in aqueous solutions at 25°C. *J. Phys. Chem. B* **102**, 4193 (1998).
36. D.K. Belashchenko. Application of the embedded atom model to liquid metals: Liquid sodium. *High Temp.* **47**, 494 (2009).
37. D.K. Belashchenko. Computer simulation of liquid zinc. *High Temp.* **50**, 61 (2012).
38. J. Frenkel. *Kinetic Theory of Liquids* (Dover, 1955).
39. A.R. Dexter, A.J. Matheson. Elastic moduli and stress relaxation times in liquid argon. *J. Chem. Phys.* **54**, 203 (1971).
40. *CRS Handbook of Chemistry and Physics: A Ready-Reference Book of Chemical and Physical Data.* Edited by R.C. West (CRC Press, 1996).
41. *Physical Acoustics. Vol. 1. Principles and Methods.* Edited by W.P. Mason (Academic Press, 1964).
42. C. Klieber, D. Torchinsky, T. Pezeril, K. Manke, S. Andrieu, K.A. Nelson. High frequency longitudinal and shear acoustic waves in glass-forming liquids. *J. Phys.: Conf. Ser.* **214**, 012033 (2010).
43. R. Hartkamp, P.J. Daivis, B.D. Todd. Density dependence of the stress relaxation function of a simple fluid. *Phys. Rev. E* **87**, 032155 (2013).
44. P.S. van der Gulik. The linear pressure dependence of the viscosity at high densities. *Physica A* **256**, 39 (1998).
45. D.K. Belashchenko, N.Yu. Nikitin. The embedded atom model of liquid cesium. *Russ. J. Phys. Chem. A* **82**, 1283 (2008).
46. W. Schommers. Pair potentials in disordered many-particle systems: A study for liquid gallium. *Phys. Rev. A* **28**, 3599 (1983).

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ПРОЯВИ ІСНУВАННЯ КОЛЕКТИВНОГО ПЕРЕНОСУ В АТОМАРНИХ РІДИНАХ ТА РІДКИХ МЕТАЛАХ

В роботі досліджується прояв колективних складових теплового руху “частинок” (молекул та іонів) у поведінці їх ефективних радіусів. Встановлено конкретний вигляд температурної залежності ефективних радіусів молекул та іонів. Демонструється їх добре узгодження з гідродинамічними радіусами, що визначаються за формулою Айнштайна–Стокса. Звертається увага на відмінності між значеннями радіусів частинок, що використовуються для опису термодинамічних та кінетичних властивостей рідин.

Ключові слова: тепловий рух молекул, колективний перенос, коефіцієнт самодифузії молекул рідини.