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Short Communication

Some Abnormal Properties of Water in the Cluster Model

G.A. Melnikov*, N.M. Ignatenko†, V.G. Melnikov

Southwest State University, 94, 50 let Octyabrya Str., 305040 Kursk, Russia

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In the framework of the cluster model developed by the structure of liquids for the anomalous dependences of the speed of sound and thermal conductivity of water temperature along the liquid-vapor equilibrium are explained.

Keywords: Speed of sound, Clusters, Cluster model, Critical point, Noble gases, Water.

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A great variety of theoretical and experimental work is devoted to the study of abnormal structural and thermodynamic properties of water, and in these latter days their number is continuously increasing [1, 2]. The speed of ultrasonic waves (ultrasound waves) in the "normal" liquids decreases monotonically with increasing temperature along the saturation line, in the water in the separation of the melting point the speed of the ultrasonic waves at first increases, reaches a maximum value at temperature of 74 °C, and only then there is a decrease in the speed of ultrasound waves with increasing temperature. This is the acoustic anomaly of water. The dependence of the thermal conductivity from temperature for the water saturation line has a similar anomaly, but the position of the maximum thermal conductivity refers to a temperature about 150 °C.

The cluster model of the structure of liquids, developed by the authors [3-5] allows us to explain and to describe the behavior of the sound speed and thermal conductivity of the water along the liquid-vapor equilibrium and on isotherms. The cluster model assumes the existence of cluster formation in the liquid and the equilibrium distribution of clusters on the number of members is set with probability density function

$$f(x)=\frac{\lambda^{\alpha}}{\Gamma(\alpha)}Z^{\alpha-1}e^{-\lambda Z}, \quad (1)$$

where λ – is the scale parameter ($\lambda > 0$), α – is the order of the distribution ($\alpha > 0$), $\Gamma(\alpha)$– is Gamma function, z – is the number of particles in cluster.

The average number of particles in the cluster is defined by the formula [3-5]

$$\bar{Z}=\int_0^{\infty} Z\cdot f(Z)dZ=\frac{\alpha}{\lambda}=\pi^2\eta\exp(\eta), \quad (2)$$

where η – is the ratio of atomic packing and defined as ratio of the particle volume to the total volume per particle in matter

$$\eta=\frac{\upsilon_{atom}}{\upsilon}=\frac{\pi\sigma_0^{\,3}}{6\upsilon}, \quad (3)$$

where σ_0 – is the effective diameter of the molecule of the substance.

The molecular packing in liquids cannot exceed a value of 0.75 near the melting point of the substance and its value is limited at the critical point ηc = 0.13-0.22.

For ideal and real gases discharged formula to calculate the speed of sound is given by

$$u=\sqrt{\gamma\frac{kT}{m_0}}=\sqrt{\frac{i+2}{i}\frac{kT}{m_0}}, \quad (4)$$

where i – is the number of degrees of freedom of the molecule, m_0 – is the mass of the molecule.

In liquids within the scaling theory with the formula for calculating the average number of particles $\bar{Z}$ in the cluster (2) the ratio of the speed of sound is represented by the formula

$$u=a\sqrt{\frac{i+2}{i}\frac{kT}{m_0}}\cdot\bar{Z}^{n_1}, \quad (5)$$

where α and n_1 – are empirical constants.

On the assumption that the critical point $T = T_c$ the number of degrees of freedom of the molecule remains the same and equals to i, the number of particles in a cluster at the critical point is $\bar{Z}_c$, the formula (5) can be written in the reduced form

$$u=u_c\sqrt{\frac{T}{T_c}}\cdot\bar{Z}_*^{n_1}, \quad (6)$$

here u_c – is the speed of sound at the critical point of the liquid-vapor, $\bar{Z}_*=\bar{Z}/\bar{Z}_c$ – is a reduced number of particles in the water cluster.

The resulting ratio (6) to calculate the speed of ultrasonic waves in liquids is capable to describe the abnormal behavior of this quantity in the water along the liquid-vapor equilibrium with error ± 2 %. Empirical constants of the equation (6) for water were found to be equal to: the speed of the ultrasonic waves at the critical point u_c = 186.04 m/c, n_1 = 1.625.

* MelnikovGA@mail.ru
† inmkstu@bk.ru

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For the coefficient of thermal conductivity in the framework of the rigorous kinetic molecular theory to the first approximation , the following relation is right [6]

$$K = \frac{25}{32}\left(\frac{\sqrt{\pi m_0 kT}}{\pi\sigma_0^2\Omega^{(2,2)*}}\right)\frac{C_v}{m_0}, \quad (7)$$

where m_0 – is the mass of the molecule, σ_0 – is its effective diameter , T – is the absolute temperature, c_v – is isochoric heat capacity, $\Omega^{(2,2)*}$ – is the value indicating the difference between any molecular model of an idealized sphere model.

In the framework of the cluster model the thermal conductivity of the fluid K present value, similar to (6)

$$K = K_c\sqrt{\frac{T}{T_c}}\left(\frac{\bar{Z}}{\bar{Z}_c}\right)^{n_2}, \quad (8)$$

where n_2 – is the empirical constant, K_c – is thermal conductivity of the fluid at the critical point.

The experimental studies of the thermal conductivity of water along the liquid-vapor equilibrium detect "abnormal" behavior of this quantity, existing at an inflection point on the graph of thermal conductivity on temperature on the saturation line. The kind of dependence $K = f(T)$ is shown in Figure 1 by the solid line - calculation by formula (8), * – experimental data [10]. Calculation error is ± 5 %. The exponent of the water n_2 was found to be $n_2 = 0.765$, the value of the thermal conductivity at the critical point is $K_C = 280$ mW/mK.

Based on the limited experimental data for these quantities two empirical constants in the theoretical ratios are determined, thus we have the opportunity to predict the temperature and pressure dependence of the speed of ultrasonic waves and thermal conductivity overthe entire range of state parameters of liquid.

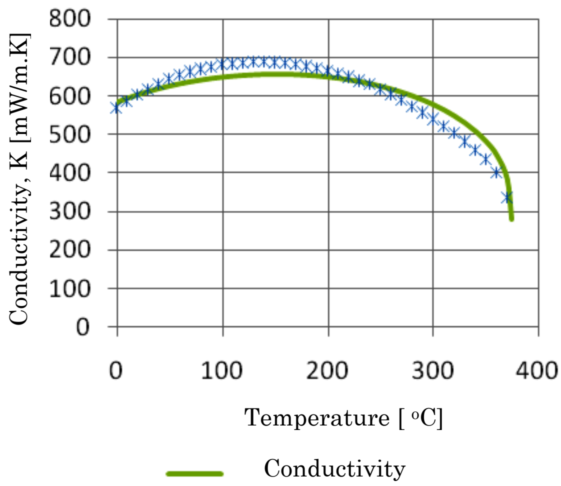

Fig. 1 - Dependency of the factor thermal conductivity from temperature on lines of the saturation for water

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