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PHENOMENOLOGICAL MODEL OF DISTRIBUTION OF WATER MOLECULES UNDER NORMAL CONDITIONS OR IN A SUPERCRITICAL STATE

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The report briefly describes the results of studies of water properties in the supercritical state (SC) or under normal conditions, which are based either on the concept of energetically preferred variations of short-range order or on the results of numerical modeling. The configuration of electron shells of a water molecule under normal conditions is described. It is proposed to consider that water molecules in the equilibrium state are grouped into hexagonal close-packed and face-centered cubic packings are in sedentary positions that can exist in water simultaneously and quickly replace each other. It is shown that the proposed model describes the maxima of the pair correlation function of water under normal conditions. A conclusion is made on the applicability of the proposed model for describing the properties of water.

Water is the most common substance on Earth, which has many applications.

One of the important applications is its use as a coolant in IV generation nuclear reactors. It is assumed that heat and mass transfer in these reactors will be carried out by supercritical (SC) water. This is explained by the fact that water in the SC state is a good heat carrier. However, along with high thermophysical characteristics, SC water is also a good solvent, which imposes certain requirements on its use. A study of its dissolving properties was carried out, for example, in [1], where encouraging experimental data were obtained on the corrosion resistance of 12X18H10T austenitic steel samples under mechanical stress and accelerated electron irradiation after 500-hour *in situ* exposure in a SC water convection loop. The effect of the absorbed dose and the level of mechanical stress on their general corrosion stimulated by electron beam irradiation is described. The composition and microstructure of the corroded surface are discussed with emphasis on the effects of irradiation and mechanical stress on the stability of the protective coating, on intergranular corrosion and on the occurrence of crack precursors.

To understand the thermophysical and corrosion properties of SC water, it is necessary to know the molecular structure of water both under normal conditions and in the SC state. However, there is no established physical model in the scientific literature that explains the molecular structure of liquid water and its high dissolving capacity in the SC state. For example, there is a new approach to describing the structure of liquid and SC water based on the concept of energetically preferable short-range order variations [2]. The validity of the proposed approach was tested on phenomena that are not yet understood but are observed during the transition of liquid water to a supercritical state. According to the results of the work, the SC state of water is a state to which the concept of "liquid-like" is hardly applicable at high pressures or temperatures. Under these conditions, it is most likely a microheterogeneous mixture of "gas-like" and "liquid-like" configurations of molecules, quickly replacing each other. Although the authors of the article note its controversial nature, in their opinion, such an approach could initiate a useful scientific discussion.

Another approach to describing the structure of water in the sub- and supercritical state is associated with numerical modeling and comparison of the obtained results with inelastic X-ray scattering data [3]. The studies have shown that hydrogen bonds in water do not disappear with increasing temperature but only undergo quantitative changes towards a decrease. It is shown that near the supercritical point, where the density of water is very low, small clusters predominate, mainly dimers and trimers, but many molecules do not have hydrogen bonds. However, it can be assumed that in SC water, as a result of a change in the number of hydrogen bonds with increasing temperature and pressure, it is possible to form not only small clusters (dimers and trimers), but nanoclusters, which are formed as a result of the reconnection of chemical bonds. For example, in [4], models are proposed for the formation of large nanoclusters of a flat or volumetric configuration in carbon dioxide in the SC state. However, the studies described above on the molecular structure of water under normal conditions or in the SC state are based on numerical models for calculating the formation of clusters, but they are not based on physically substantiated patterns.

The purpose of this report is to present the main approaches to propose a physically based model of the structure of water in the normal and supercritical states.

This report provides a brief description of the results of studies of the properties of water in the liquid and supercritical states.

A generally accepted description of the configuration of the electron shells of a liquid water molecule under normal conditions is given, which is important for further analysis of the molecular structure of water taking into account the dipole-dipole and spin-spin interactions.

The presentation of the phenomenological model of the structure of water is based on the analysis of the concept of energetically preferred variations, which is consistent with the concept of [2]. The proposed model uses a description of the distribution of water molecules in space under normal conditions in the arrangement of molecular spheres (MS) of water in a dense layered packing. In this case, the distribution of MS is proposed to be considered as a sequence of monomolecular layers MS, between which a separating layer can be located, similar to the boundary surface layer of MS. A comparison of the proposed phenomenological model of MS distribution with the pair correlation function of water under normal conditions is given. The result of such a comparison can be summarized by the following statements.

In the equilibrium state, MS are grouped into hexagonal close-packed (HCP) and face-centered cubic (FCC) packings, which can be present in the bulk of water simultaneously and quickly replace each other.

In the bulk of water, MS can contact the walls of the vessel and form a boundary surface layer of MS. This boundary surface layer of MS is a monomolecular layer of water with the densest packing of MS, where the distance between the centers of MS is about 2.8 Å.

In the bulk of water, due to the presence of a surface film of equilibrium air bubbles or vapor bubbles, surface layers of MS similar to the boundary surface layer of MS can also be present.

The distances from the test MS to the MS of the second and third rows of HCP or FCC packings in the boundary layer are of the same order. Therefore, the maxima of the pair correlation function are superimposed and, due to incomplete coincidence, are blurred and form a half-width that is greater than the half-width of the first maximum.

The subsequent maxima of the water correlation function are in full agreement with the data of the proposed model, which indicates its applicability.

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