

The Nature of Phase Transitions: "Water - Ice" and "Ice - Water"

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When cooling, water crystallizes into a structure of lower density. If the crystal volume increases by 3-5 and even 10 % in common liquids at melting, the ice volume decreases by 7.988 %.

This anomalous phenomenon remains unexplained to the present. There are many experimental and theoretical studies devoted to the investigation of the physical-chemical properties of water. However, one has not solved all of the mysteries of water.

The theory of electron-oscillatory interactions, the Yan-Taller theory, considers the interaction of electron orbitals of neighbor molecules which determine the mutual location of atoms in molecules and crystals. Since Yan-Taller theory is based upon short-range order, it may be applied to liquids as well. The interaction of two neighbor molecules of water and the orientation of electron orbitals of oxygen in two cases (a – in the ice; b – in the water) is shown in work by Antonchenko and Malafaev. The interaction of overlapping orbitals in the dimer has a repulsive character. These are the key interactions between nearest molecules of water [Antonchenko; Zacepina; Bersuker; Malafaev]; the dynamics of the process have not been studied.

The present work makes an attempt to explain the phase transitions for water-ice and ice-water on the atomic molecular level. It is observed that molecular localization begins at 0 °C. These localized molecules are on the lowest energy levels in the energy spectrum. A further cut-off of the heat supply increases the number of localizing molecules. This process goes on at 0 °C until the whole system crystallizes. The ice volume increases by 7.988 %; this happens because the structure loosens owing to the revolving of dipole molecules on their axis by hydrogen bonds, amplifying as the heat energy falls when a supply of heat is cut off.