Thermodynamic, dynamic and structural anomalous behavior in confined water

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ABSTRACT

Using molecular dynamic simulations we study a waterlike model in two different confinements: between two fixed plates and in a nanotube. We analyze the changes on density, diffusion and translational order parameter anomalies of the confined system in relation to the bulk. For the confinement between two plates we study the systems with formation of three well-defined layers with plates separated by d* = 5.5, 6.0 and 6.3. In these cases, we observe that the Temperature of Maximum Density (TMD line) shifts to lower temperatures, higher densities and higher pressures, except for d* = 6.3, that shifts slightly to lower pressures. The others anomalies follow the density anomaly, presenting a similar shifting. The structure was studied analysing each layer separately through the radial distribution function and the translational order parameter. We also calculate the lateral diffusion coefficient using the mean square displacement. The same analysis is done for d* = 4.2, that shows a structure of two contact layers, without middle layer. In this case, the solidification of the contact layers occurs more easily because the strong confinement of the plates. A peculiar system, corresponding to d* = 4.8, shows density and diffusion anomalies at very low temperatures. The perpendicular pressure as function of temperature has minimums and changes on phase diagram of perpendicular pressure as function of density, both behaviors did not see in other cases.

It can be associated with the density anomaly and changes on structure of the middle layer. The location of the anomalies depends strongly on the separation d* and the number of layers formed between the plates. For the nanotube channel we observe that the diffusion coefficient grows with the decrease of the channel radius for radius below a certain threshold.