Geophysical Research Abstracts
Vol. 20, EGU2018-12937, 2018
EGU General Assembly 2018

Temperature Dependence of the Surface Tension of Supercooled Water determined by Molecular Dynamics Simulations

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The surface tension of water (σw) influences the equilibrium between aqueous droplets and water vapor as well as activation of cloud condensation and ice nuclei in the atmosphere. The temperature dependence of the surface tension of liquid water above 273.15 K (0 °C) has been studied extensively and is well constrained by experimental data. However, controversy exists over the dependency in the supercooled temperature regime, especially on the existence of the "second inflection point" in the experimental data of supercooled water. In fact, the cause of change of σw along with temperature has not yet been fully understood even at temperature above 273.15 K. Here, we use molecular dynamics simulations to study the surface tension of water at different temperatures (σw(T)), ranging from 198.15 K to 348.15 K. As expected, we observed an increase of σw(T) with decreasing temperature. Above 273.15 K, the simulated surface tension correlates well with the prediction from the International Association for the Properties of Water and Steam (IAPWS). Further decreasing temperature, no "second inflection point" is found until ~250 K. At around 240 K, the surface tension begins to deviate significantly from the extended IAPWS curve and shows an amplified temperature dependence. By separating enthalpic and entropic contributions to σw(T) over the studied temperature range, we further explored the possibility of a "second inflection point" of σw(T). Energetic analyses show that the change of σw(T) along temperature is found to be an entropy-driven process above 240 K, but an enthalpy-driven process below it. Furthermore, we find that the increase of σw(T) with decreasing temperature has a nearly linear correlation with the decrease of the interfacial width, and we interpret this behavior in term of capillary wave theory which is found to describe the dependence of interfacial widths on surface linear dimension and temperature. Deep in the supercooled regime, a compact water layer in the interface (i.e. the density is higher than the bulk water density) is detected. Our findings should help to understand nucleation phenomena in the atmosphere from water vapor at strongly supercooled temperature.