The surface tension of small drops

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An effective method of nanoparticles production is the condensation of nanodrops from supersaturated vapor. Nucleation, formation of critical nuclei, is the first stage of such condensation. The surface tension of small drops is the most impotent parameter in the nucleation theory, as it determines the work of the critical nuclei formation.

In our report the results of molecular dynamics calculations of small drops are presented. The equilibrium states of Lennard-Jones molecular system containing one small drop of $50 - 4000$ molecules and the saturated vapor have been prepared. The density profiles, the Irving-Kirkwood pressure tensors, the chemical potentials of the systems, the mechanical and Gibbs's surface tensions have been calculated. The difference between the mechanical definition of surface tension and the Gibbs's one is in the fact, that in the first case the real drop is replaced by the spherical container, the pressure inside the container being chosen as equal to the pressure in the center of the drop, and in the second case the pressure inside the container corresponds to the pressure in the bulk liquid with chemical potential equal to that in the calculated system.

The dependence of the surface tension of small drops on the equimolar radius and temperature has been calculated. It was found that the mechanical surface tension is different from the Gibbs's surface tension for drops of $50 - 2000$ molecules and is equal for drops of more than 2000 molecules. It is shown that both the mechanical and Gibbs's surface tensions decrease with the decrease of the equimolar radius of the drop, and reach zero at the same R_0 depending on temperature. The dependence of the ratio of the surface tension of the drop to the surface tension of the flat surface liquid-vapor (σ/σ_∞) on the ratio of the equimolar radius of the drop to R_0 is a universal function.