# Determination of Nanoparticles Surface Tension from Experimental Data on Homogeneous Nucleation of Ibuprofen Vapors

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## Introduction

Past years of investigations have shown that properties of nanoscaled matter can dramatically differ from that of a bulk matter. The thermodynamic properties of interphase boundary layer can be fully characterised by the state function called surface tension, $\sigma$. In Gibbs rigorous theory surface tension is the function of curvature radius. Therefore, the information of surface tension dependence on nanoparticle radius $R$ is very important when investigating colloid systems (i.e. processes of formation, aging, stability). Unfortunately, it is not easy to measure nanoparticle surface tension in direct experiments. However, it is possible to estimate surface tension of nanoparticles by the means of i.e. MD simulations, but only for simple systems (for example, LJ fluids). On the other hand the homogeneous nucleation rate is a function of surface tension. Therefore experimentally determined homogeneous nucleation parameters (nucleation rate, temperature, supersaturation ratio) can be used for $\sigma(R)$ dependence evaluation. Recently a new rigorous formula for homogeneous nucleation rate has appeared (Vosel *et al*, 2009). This formula takes into account not only the dependence $\sigma$ on nanoparticle radius but also translation-rotation movement of a critical nucleus.

The goal of this work was to determine homogeneous nucleation parameters for ibuprofen (popular NSAID), and to determine critical nuclei surface tension.

## Methods

In our experiments we utilized laminar flow horizontal nucleation chamber. It consisted of a quartz tube with an external cylindrical heater. An inert carrier gas (argon, 99.999% purity) entered the chamber and passed through heated zone of the tube. A crucible with a ibuprofen racemate (Aldrich) was located in the maximum inner temperature zone of the heated area. During typical experiment the substance evaporated from the crucible. A gas flow containing ibuprofen unsaturated vapors entered a cool zone of the chamber. As gas cooled vapors became saturated first, then supersaturation ratio increased and homogeneous nucleation occurred in some area of the chamber. New formed critical nuclei grew fast due to vapor condensation on them.

The number concentration and average diameter of aerosol particles at the exit of the chamber were measured by automatic diffusion battery (ADB). In order to obtain the approximate location of nucleation zone a new “supersaturation cut-off” technique was used. 3D supersaturation and temperature profiles inside the chamber were obtained through experiments as well as computer simulations. Experimental data was used to calculate homogeneous nucleation rate. Then using the rigorous formula (Vosel *et al,* 2009) surface of tension of critical nuclei was obtained as well as their radius $R$.

## Results

It was found that the surface tension of 1.6 nm radius ibuprofen critical nuclei is about 1.06 times larger than surface tension of bulk ibuprofen ($24.38 \cdot 10^{-3}$ N/m at the temperature of nucleation). This results correspond to temperature of nucleation equals to 318K, supersaturation ratio 11 and homogeneous nucleation rate $10^7$ $cm^{-3}s^{-1}$. Critical nucleus of 1.6 nm radius contains approximately 36 ibuprofen molecules.

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