# CONDITIONS FOR CREATING THIN LIQUID LAYERS AT THE CONTACT SURFACE OF TWO OTHER LIQUIDS

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*Summary:* The design of new technologies, for manufacturing the nano – structured materials is one of the important tasks of the contemporary materials science. The use of emulsion droplets as templates for producing nanostructures out of solid particles, suspended in the liquid phase is already under development. In the present work we investigate the possibility of using a liquid film instead of solid particles. To simulate the behaviour of the liquids we apply the Molecular Dynamics simulation technique. Since the behaviour of the liquids depends mainly on the interaction potentials of the molecules, we look for combination of the interaction potentials, which might produce the required liquid film at the surfaces of the emulsion droplets.

## INTRODUCTION

The design of new technologies, making it possible to manufacture the nano – structured materials is one of the most important tasks of the contemporary materials science. The technologies, utilizing the emulsion droplets as templates for producing nanostructures out of solid particles, suspended in the liquid phase, seem very promising; work on developing such technologies is progressing fast [1]. It seems however conceivable, that even smaller structures could be obtained, if instead of solid particles a liquid film was utilized.
In the present research we investigate the conditions necessary for producing a liquid film at the interface of two nonmixing liquids.

## SIMULATION DETAILS

To simulate the behaviour of the three liquids we apply the Molecular Dynamics simulation technique. For the detailed calculations we use the program "MOLDY" [2].
Since, at the molecular level, the behaviour of the liquids depends, in the first place, on the interaction potentials between the molecules [3], we look for the combination of the interaction potentials, which might produce the required liquid film at the surfaces of the emulsion droplets. We perform a number of simulation runs, assuming different interaction potentials. The liquids used for simulations are actually model liquids with desired properties, not the real ones. Still, the information, relevant for the technology, is obtained in this way. Having the information on the required interaction potentials one can look for the real liquids, fulfilling these requirements.

## PRELIMINARY RESULTS

The aim of the preliminary calculations was to simulate formation of the liquid droplet in a vacuum and in another, nonmixing liquid. We placed a number of liquid molecules in a recangular lattice and allowed them to move freely with velocities, corresponding to a prescribed temperature.
At the beginning we tried, for simplicity, to use the Simplified Water Model (SWM) – a liquid of spherically symmetric molecules, interacting with each other only through the Lennard – Jones potential, the same as that for water. Such molecules, placed in a vacuum, spread uniformly in the whole simulation domain. To form a well – defined droplet it was necessary to use more realistic model of the water molecule (TIPS2, [4]), taking into account the electrostatic dipole interactions. Such interactions, on top of the Lennard – Jones potential, are the most important factor influencing the behaviour of water.
The initial configuration of the water molecules, taken for simulation, was actually very far from spherical. This produced oscillations of the shape of the droplet, visible for certain amount of time. The frequency of these oscillations was comparable to the mean molecular speed divided by the diameter of the droplet.
To simulate the formation of a liquid droplet, immersed in another, nonmixing liquid, we first tried the SWM molecules, however without electrostatic dipole interactions certain amount of mixing was always present. To produce a liquid droplet successfully we had to immerse the SWM liquid, (which now could represent oil) in water described by the TIPS2 model.
The following pictures present some of the obtained results.

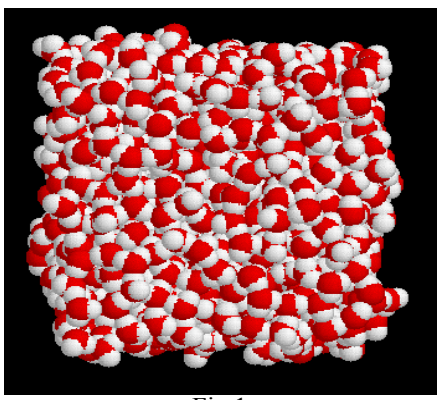

Fig.1.

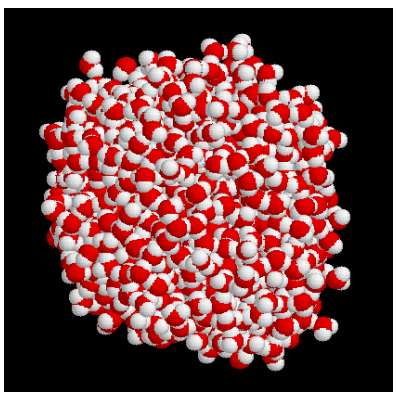

Fig. 2.

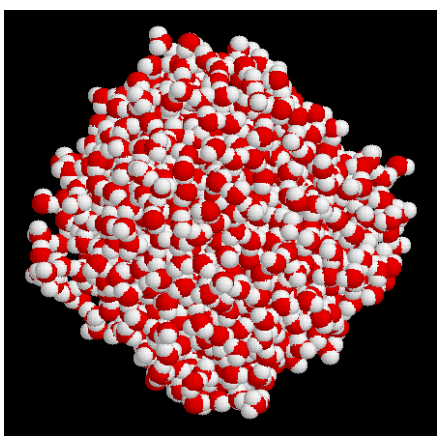

Fig. 3.

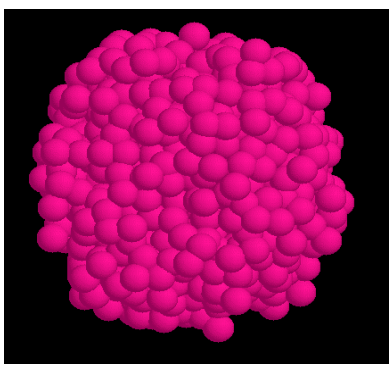

Fig. 4.

Fig. 1. Water droplet in vacuum short after start of simulation.
Fig. 2. The same after ¼ of the oscillation period.
Fig. 3. The same after ½ of the oscillation period.
Fig. 4. Oil droplet immersed in water after equilibration.

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