Annex 5

CREATING A THIN LIQUID LAYER AT THE CONTACT SURFACE OF TWO OTHER LIQUIDS

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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, using the emulsion droplets as templates to produce nanostructures out of solid particles suspended in liquid phase are under development [1]. It seems conceivable, that even smaller structures could be obtained if a liquid film was used instead of solid particles. In the present research we investigate the conditions necessary for producing such liquid film at the interface of two other, immiscible liquids.

METHOD

In the investigated method of producing nanomaterials we used emulsion consisting of water and oil. Diameters of the oil droplets were very small, so we could not use the classical, continuum methods to describe processes in liquids. To simulate the behavior of the three liquids we applied the Molecular Dynamics simulation technique [3]. For the detailed calculations we used the program “MOLDY” [2].

RESULTS

For calculations the molecular model of water, TIPS2 [4] was used. To test its behavior, formation of water droplet in vacuum was simulated (Fig.1, 2). The molecules initially placed in a rectangular lattice, after some time created a spherical shape, and later the beginning of evaporation was observed.
To the test the oil molecules, formation of an oil droplet in water and water droplet in oil was simulated (Fig.3, 4). The obtained oil droplet in water was more stable than the water droplet in oil, which agrees with macroscopic observations.

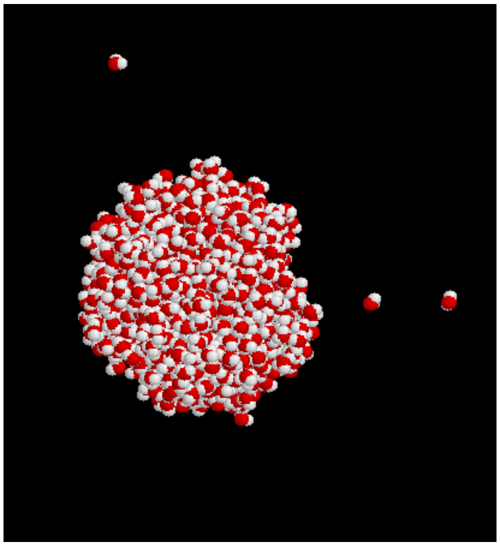

Fig.1.

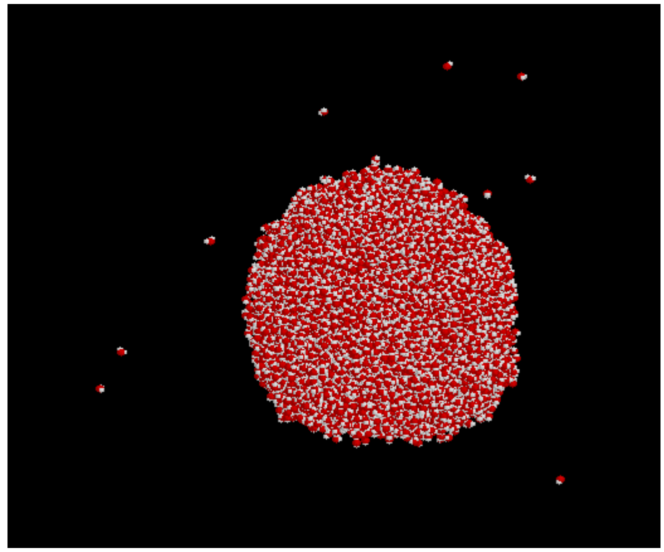

Fig.2.

Fig.1. Water droplet in vacuum (1000 molecules, diameter of the droplet = 3,8 nm).
Fig.2. Water droplet in vacuum (10648 molecules, diameter of the droplet = 8,4 nm).
Evaporating molecules can be seen in both pictures.

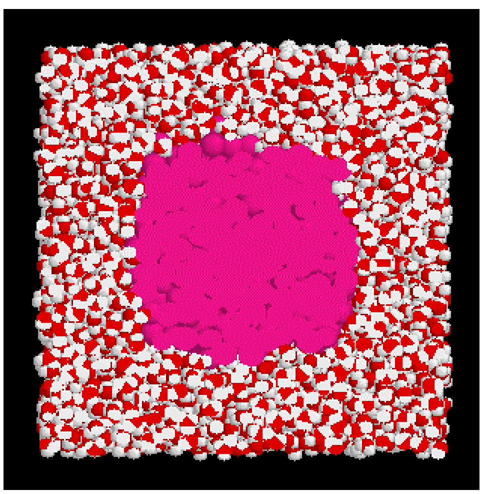

Fig.3.

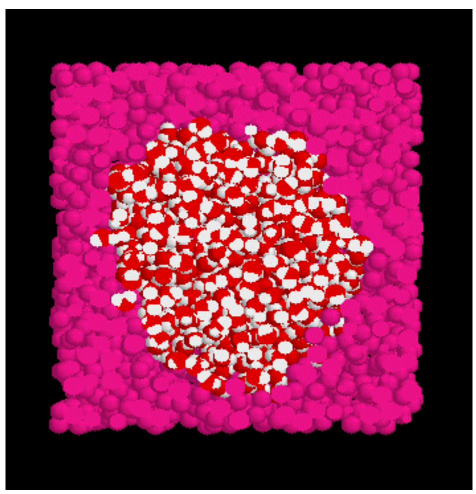

Fig.4a.

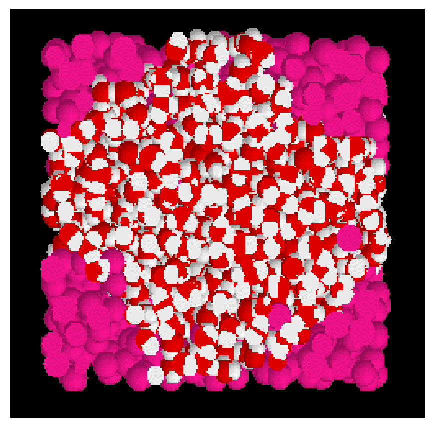

Fig.4b.

Fig.3. Oil droplet in water (d=3,7 nm).
Fig.4a,b. Destabilization of water droplet in oil (d=3,8).

To simulate interactions between three liquids we used the same models of water and oil. The third component was similar in its structure to soap, whose molecules consist of two parts – resembling the molecules of oil and water. After some modification of the model of the third component (increasing the length of its molecules), the thin film between layers of oil and water was obtained (Fig.5).

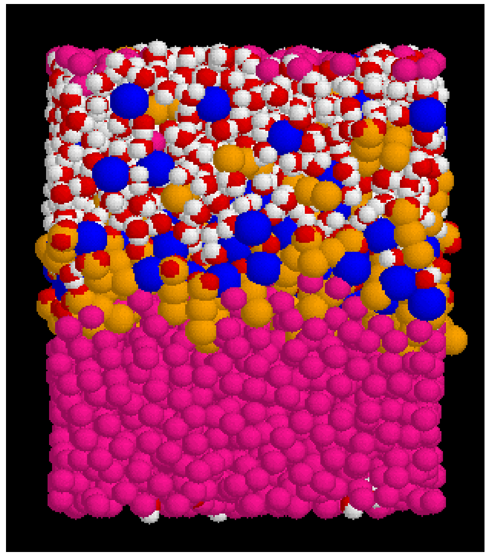

Fig.5. The thin film of „soap" between oil and water.

For more information see: *„Creating a thin liquid layer at the contact surface of two other liquids"* A. Slowicka, Z. Walenta, Euromech colloquium n°472: "Microfluidics and Transfer**"** September 6-8, 2005, Grenoble, France.

LAST RESULTS

The last simulations were aimed at obtaining the layer of solid particles at the interface between water and oil. At first, a suspension of carbon particles in oil was produced (Fig.6a,b). To force carbon to produce the layer at the interface, the parameters of the interaction potential of carbon ("quasi-carbon") were changed, but these changes did not have any significant influence upon the process (Fig.7a,b).

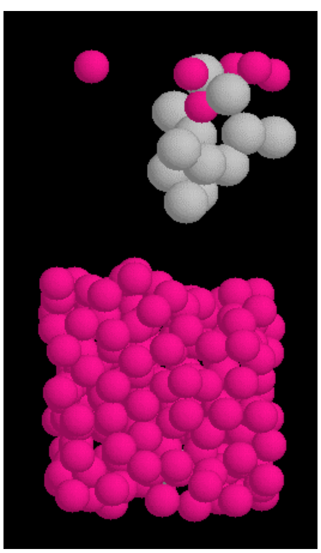

Fig.6a.

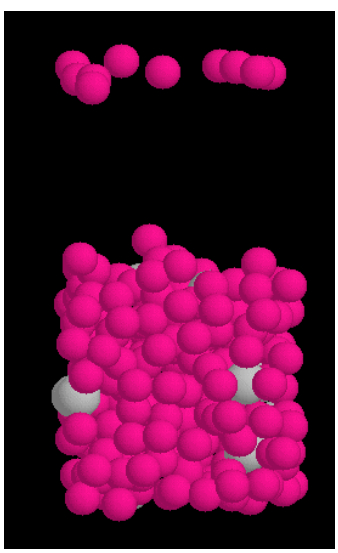

Fig.6b.

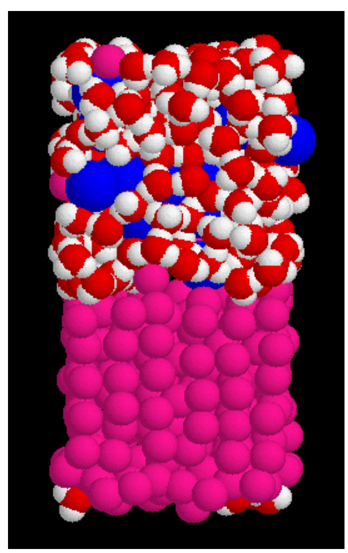

Fig.7a.

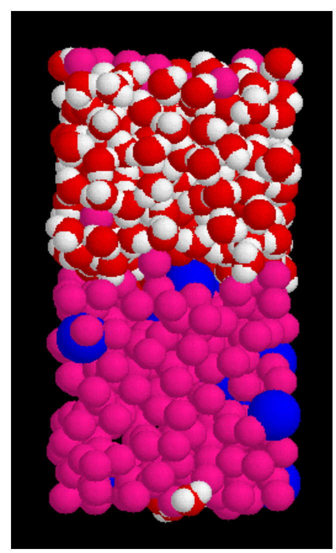

Fig.7b

Fig.6a. Carbon dissolved in water (molecules of water are transparent) – start of the simulation.
Fig.6b. Carbon dissolved in oil – end of the simulation.
Fig.7a,b. The same simulation for “quasi-carbon”.

Acknowledgements

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References

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