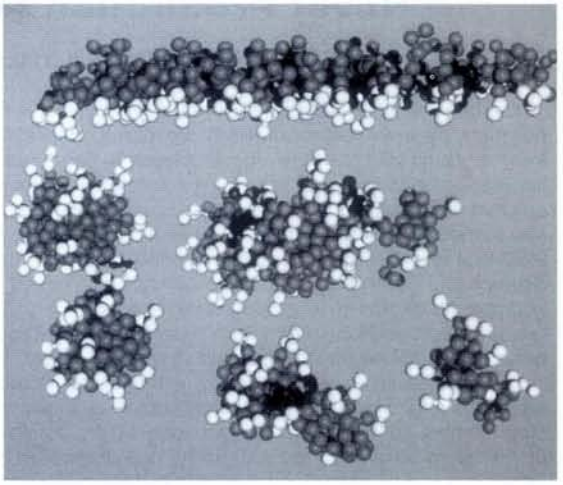
Surfactants Can be Modelled

DYNAMICAL PROCESSES IN MICELLES REPRODUCED



Snapshot of part of the surfactant/water system. For clarity only the surfactants are shown; the white spheres are the hydrophobic segments. A monolayer has formed at the interfaces of micelles in the water phase.

Amphiphilic molecules such as surfactants, lipids, or detergents have an affinity for both water and oil. The polar head of the molecule is hydrophilic, while the hydrocarbon chain is responsible for the affinity for oil. Dissolved in water, surfactants tend to aggregate in micelles. Micelles are simple forms of self assemblies. At higher surfactant concentration, various different assemblies such as bi-layer, cylindrical micelles, vesticles, and other structures may form. Despite the importance of these assemblies in various processes — ranging from the transport of molecules through upper-cell membranes to the removal of stains in a washing machine — our knowledge of self-assembly at a molecular level is still very poor. Computer simulations may contribute to a better understanding of these fascinating systems.

In our simulations we have used a simple water surfactant/model. The starting points of the model are: oil and water do not like each other, and a surfactant is an amphiphilic molecule, *i.e.*, one side of the molecule likes oil but dislikes water, the other side likes water but dislikes oil. Both water and oil particles are modelled with a truncated Lennard-Jones potential. The truncation of the potential is made dependent on the type of interaction such that the oil-water interactions are purely repulsive and the water-water and oil-oil interactions attractive. A surfactant is made up by several oil and water particles connected *via* harmonic springs [Smit B., *et al., Nature* **348** (1990) 624; *J. Phys. Chem.* **95** (1991) 6361; *Langmuir* (in press) 1992]

Computer simulations on a water/surfactant system with 32 000 particles were performed on a network of 400 transputers using a parallel molecular dynamics algorithm [Esselink, K., Smit, B., and Hilbers, P.A.J., *J. Comp. Phys.* (in press) 1992]. The simulations were started from a completely random distribution of surfactant. A snapshot of a small part of the equilibrated system is shown in the figure. It demonstrates that micelles have formed spontaneously.

One of the remarkable results of our simulations is that we can observe the dynamical processes in a micellar solution. The typical time scale of these processes have been determined experimentally. For example, the time scale for individual surfactants to leave a micelle is 10^{-8} to 10^{-6} s, the fusion of two micelles takes 10^{-5} to 10^{-4} s, and the typical lifetime of a micelle is of the order of 10^{-3} to 10^{-1} s. These time scales are clearly (far) out of the range accessible by simulations on realistic models, where the maximum simulation time is of the order of 10^{-9} s.

It turned out that our simple model does show these phenomena in a time span that is accessible in a computer simulation. This allows us to use molecular dynamics to study the dynamical processes that are of importance in many biological and industrial applications.

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Orientational Phenomena in Polymers

25th EUROPHYSICS CONFERENCE ON MACROMOLECULAR PHYSICS

St. Petersburg, Russia
6-10 July 1992

The Winter Palace in St. Petersburg

Polymers widen the range of material properties because their molecules are large; long in the case of thermoplastics. Extreme properties occur when molecules are aligned with chain connectivity along one direction. In such circumstances the familiar properties of polyethylene, for example, are much changed and it then behaves as a one-dimensional diamond, with an axial Young's modulus some 50% higher than that of steel. Such was the potential first widely appreciated a quarter of a century or so ago: it is now a reality with the increasing range of high-performance fibres and oriented polymers that are generally available in the market-place.

The Europhysics conference in St. Petersburg brought together the principal international investigators in this active field and provided a timely opportunity to review prospects and to look ahead. The chosen themes were wide-ranging, encompassing amorphous as well as crystalline systems, liquid as well as solid states, mechanisms of formation as well as resulting properties, understanding as well as knowledge. Due prominence was given to mechanical behaviour, but a notable session on conducting polymers, including a talk by P. Smith and U. Shirakawa brought much order into a particularly fast-moving area. It also emphasized that orientation improves with conductivity and mechanical behaviour in parallel, so that highly conductive systems tend to have good mechanical properties.

On mechanical aspects not only were the pioneers (Ward, Keller, Pennings, Lemstra, and others) present in person but each showed in their characteristic way the importance of current achievements and the rich potential the field still holds for the future (see box).

Scientifically, the conference was unquestionably first class, for the quality of its contributions, the discussion which was stimulated, and the personal contacts which were established and renewed. Logistically the conference was quite extraordinary. It had seemed to many that to organize any meeting in the circumstances of present-day Russia