

Thermal gradients in aqueous soft matter systems

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In many experimental situations temperature gradients play an important role. For almost one century thermogravitational columns and thermal field flow fractionation channels have been used for separation and characterization of soft matter [1]. Presently researchers design synthetic microswimmers, micromotors, or micropumps to explore possibilities to recycle waste heat using such microfluidic devices [2]. So far there is only a limited microscopic understanding of thermodiffusion or thermophoresis in simple and complex fluids. In the recent years some progress has been made for non-polar systems, but in aqueous systems the situation is complicated due to charge effects and strong specific cross interactions so that simple thermodynamic concepts fail. On the other hand a detailed understanding of aqueous systems would be valuable due to important applications in biotechnology, where the response to temperature gradients is successfully employed to monitor the reaction kinetics of large proteins with small ligand molecules. The strong sensitivity of proteins and other water soluble biomolecules is probably caused by a change in the hydration layer, which is influenced by subtle conformation changes induced by the binding of the ligand molecule. To get a better understanding we systematically investigated various small water soluble molecules, microemulsions and colloids by a holographic grating method called infrared thermal diffusion forced Rayleigh scattering (IR-TDFRS). In order to elucidate the mechanism in biomolecules we performed systematic measurements of amides, which often serve as model systems for peptide bonds, an essential structure in proteins. Using the experimental data determined for formamide we perform numerical finite-element simulations in hydrothermal pores and show that a combination of thermophoresis and convection can lead to accumulation of formamide up to concentrations where nucleobases are formed [3], which might serve as an ‘origin-of-life’ scenario. Further we study microemulsion droplets as soft colloids to investigate the relation between the interfacial tension and the Soret coefficient [4]. Other important contributions in aqueous systems are charge effects, which we study systematically for colloidal model systems. Using a theoretical model by Dhont and Briels [5] valid for spherical charged colloids with arbitrary double-layer thicknesses we are able to calculate the surface charge density of the colloid. It turns out that the surface charge density agrees well with electrophoresis measurements. The same holds for an extended model for charged colloidal rods [6].

[1] Wiegand, S., in *Functional Soft Matter*, J.K.G. Dhont, et al., Editors. 2015, Forschungszentrum Jülich. F4.

[2] Ripoll, M. and Yang, M.C., in *World Scientific Lecture Notes in Complex Systems - Vol. 12 Engineering of Chemical Complexity II* (2015) 109.

[3] Niether, D., Afanasenkau, D., Dhont, J.K.G. and Wiegand, S., *PNAS*, **113** (2016) 4272.

[4] Naumann, Ph., Datta, S., Sottmann, T., Arlt, B., Frielinghaus, H., Wiegand, S., *J. Phys. Chem. B*, **118** (2014) 3451.

[5] Dhont, J.K.G. and Briels, W.J., *Eur. Phys. J. E*, **25** (2008) 61.

[6] Wang, Z., Kriegs, H., Buitenhuis, J., Dhont, J.K.G., Wiegand, S., *Soft Matter*, **9** (2013) 8697.