

CPP 9: Crystallization and Self Assembly II

Time: Monday 14:00–16:30

Location: H48

CPP 9.1 Mon 14:00 H48

A multi relaxation time lattice Boltzmann model for amphiphilic fluid mixtures — ●SEBASTIAN SCHMIESCHEK¹ and JENS HARTING^{2,1} — ¹ICP Univ Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — ²MTP, Dept Appl Phys, TU Eindhoven, P.O.B. 513, 5600 MB Eindhoven, The Netherlands

Due to its inherent mesoscopic character and ease of implementation and parallelisation, the lattice Boltzmann method (LBM) has become a popular model for simulations of soft matter systems. However, the broadly used single relaxation time schemes suffer from restrictions, such as a fixed Prandtl number and limited numerical stability. The introduction of a multiple relaxation time model allows a differentiated treatment of the modelled physical properties overcoming part of these problems. The present work integrates a multi relaxation time (MRT) scheme to an implementation of the popular Shan Chen type LBM. The code allows the simulation of binary and ternary multicomponent systems, containing (im)miscible and optionally amphiphilic fluid species. It has been applied to study various problems like the rheology of mesophases and microemulsions or multiphase flows in microfluidic systems. Exemplary simulations of amphiphilic mixtures and basic benchmark results of the MRT scheme are presented.

CPP 9.2 Mon 14:15 H48

Testing the Renormalized One-Loop Theory for $S(q)$ in Diblock Copolymers — ●DAVID MORSE^{1,2} and JIAN QIN¹ — ¹University of Minnesota — ²University of Goettingen

We compare predictions of the renormalized one-loop (ROL) theory of correlations in block copolymers to extensive simulations of a simple bead spring model. The ROL theory is a rigorous theory of corrections to the random-phase approximation for the structure factor $S(q)$, to first order in an expansion in $N^{-1/2}$. ROL theory includes the Fredrickson-Helfand FH theory as a limiting case, in the limit of large peak-intensity, very near the ordering transition. ROL theory (but not FH theory) is found to give accurate predictions for both the peak intensity and peak wavenumber over a wide range of values of the Flory-Huggins interaction parameter χ , from $\chi = 0$ to the transition.

CPP 9.3 Mon 14:30 H48

3d versus 2d Freezing of Lennard-Jones Fluid in a Slit Pore — ●NADEZHDA GRIBOVA, AXEL ARNOLD, and CHRISTIAN HOLM — ICP, Universität Stuttgart

We present a computer simulation study of a (6,12)-Lennard-Jones fluid confined to a slit pore, formed by two structureless planes. These interact via a (3,9)-Lennard-Jones potential with the fluid particles. Walls in the system induce layering. In order to investigate the nature of the freezing transition, we perform a detailed analysis of the bond-orientational order parameter and diffusion in the layers. Varying the distance between the slit walls, we study the system accommodating from 1 to 7 layers. With increasing number of layers the behaviour changes from a quasi-2d crystallization without hysteresis and an intermediate hexatic phase to a standard 3d.

CPP 9.4 Mon 14:45 H48

Molecular Dynamics Simulations of Polymer Crystallization via Self-seeding — ●CHUANFU LUO and JENS-UWE SOMMER — Leibniz Institute of Polymer Research Dresden, 01069, Dresden

We use large scale molecular dynamics (MD) to simulate the processes of polymer crystallization with a coarse-grained model. In total we are able to simulate 1000 polymer chains made of 1000 monomers each, a system large enough to compare to experimental relevant, entangled melts. It is found that some micro crystalline domains (MCDs) can survive slightly above the apparent melting temperature after a cooling and reheating cycle. We chose the stablest MCD as a baby seed and let it grow at a constant quenched temperature. A single lamella can be formed via this self-seeding process. We observe the growth pathway and analyze the chain dynamics especially at the growth front. We thank the financial support by Deutsche Forschungsgemeinschaft (DFG) SO 277/6-1.

Selected references: [1] C. Luo and J. Sommer, *Comp Phys. Comm.* 180, 1382 (2009) [2] C. Luo and J. Sommer, *Phys. Rev. Lett.* 102, 147801 (2009) [3] J.-J. Xu, Y. Ma, W.B. Hu, M. Rehahn and G. Reiter, *Nature Materials* 8, 348 (2009)

CPP 9.5 Mon 15:00 H48

Novel method for the growth of highly crystalline P3HT thin films — ●SHABI THANKARAJ SALAMMAL¹, MARTIN BRINKMANN², PATRICK PINGEL³, ULLRICH PIETSCH¹, NILS KOENEN⁴, and ULLRICH SCHERF⁴ — ¹Solid State Physics, University of Siegen — ²Institute Charles Sadron, Strasbourg. — ³Soft Matter Physics, University of Potsdam. — ⁴Macromolecular Chemistry, University of Wuppertal.

Role of growth temperature in crystallinity of P3HT thin films have been demonstrated here. Films were prepared at RT and -30°C above the OTS treated SiO₂ substrate. X-ray diffracted intensity of -30°C grown film gained by the factor of 3 while comparing the films prepared on with and without OTS treated substrates. The degree of preferential orientation has been quantified via Chi scan, where incident and detector angle were fixed under specular condition of (100) Bragg peak. The OTS treated substrate provides a higher number of oriented crystallites than the non OTS treated one; it could be due to the possible interdigitation of OTS and P3HT polymer side chains. Diffracted intensity of -30°C grown film has one order of magnitude higher than the RT grown one. 2D x-ray diffraction pattern envisage the presence of flat and edge-on-orientation in RT grown film but flat-on-orientation is completely absent at -30°C casted one. X-ray diffraction has been confirmed by electron diffraction as well. HRTEM image envisage the presence of flat-on orientation in spin coated film. The luminescence intensity gained by the factor of two and mobility gained by one order of magnitude while comparing -30°C casted with RT, those results will be correlated with increase in conjugation length of the polymer.

CPP 9.6 Mon 15:15 H48

What controls heterogeneous nucleation of polymers at interfaces? — ●THOMAS HENZE, KLAUS SCHRÖTER, and THOMAS THURN-ALBRECHT — Martin-Luther-University Halle-Wittenberg, Institute of physics, D-06199 Halle (Saale), Germany

We here present a study of the morphology of thin films of polyethylene crystallized from melt on a number of substrates with different ability to invoke crystallization, namely mica, NaCl, SiO₂ and HOPG. Using intermittent-contact mode AFM very different structures are observed on the surface of the polymer films depending on the kind of substrate, the film thickness as well as the degree of branching of the polymer.

For very thin films (about 30 nm) on NaCl and HOPG short, edge-on lamellae oriented according to the symmetry of the underlying crystal lattice show up indicating epitaxial growth. With increasing film thickness (up to 300 nm) the preferred edge-on orientation of the lamellae remains, while the in-plane orientation tends towards one fixed direction. The morphology itself indicates a very high nucleation ability for these kind of substrates. In contrast to that on SiO₂ and mica a spherulitic structure is present showing a preferred flat-on orientation of the lamellae in the thinnest films. However, a quantitative analysis of nucleation density shows that also on these substrates heterogeneous, but non-epitaxial nucleation takes place.

CPP 9.7 Mon 15:30 H48

Local and Collective Motions in Polyolefins with Precise Alkyl Branches: a Solid State NMR Study — ●ROBERT GRAF¹, YUYING WEI², KENNETH B. WAGENER², and HANS WOLFGANG SPIESS¹ — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²University of Florida, Gainesville, Florida (USA)

In linear polymers, such as polyethylene (PE), chain branches change the local mobility and have pronounced effects on the mechanical properties, such as processability and drawability. In many previous studies, the irregular distribution of the branching sites along the main chain caused an uncertainty of the branching influence on morphology, chain dynamics, as well as other physical properties. Here results from investigations of dynamic processes in crystalline regions of PE samples with regular spaced methyl branches. By deuteration of the methyl branches, the molecular dynamics of the defect site can be studied selectively via 2H NMR methods, whereas molecular reorientations of the polymer chain between the branching sites can be monitored separately via 13C chemical shift anisotropy measurements. Combining these results with studies of local conformations, a twist motion can be identified, which is localized at the branching sites for a spacing of more than twenty CH₂ units between subsequent branching points.

In methyl branched PE samples with shorter spacing, a collective dynamic process can emerge from this twist motion, which ultimately leads to the formation of a rotator phase.

CPP 9.8 Mon 15:45 H48

Single-Molecule Force Spectroscopy of Supramolecular Heterodimeric Capsules. — •TOBIAS SCHRÖDER^{1,2}, THOMAS GEISLER², BJÖRN SCHNATWINKEL², DARIO ANSELMETTI¹, and JOCHEN MATTAY² — ¹Department of Physics, Experimental Biophysics & Applied Nanosciences, Bielefeld University, — ²Department of Chemistry, Organic Chemistry I, Universitätsstrasse 25, 33615 Bielefeld, Germany

Despite the rich information accessible, atomic-force single-molecule force spectroscopy (AFM-SMFS) has scarcely been employed to analyze the bonding between building blocks of complex supramolecular structures [1]. After the pioneering work by Eckel et al. [2], we investigated the multiple bonding interaction in a supramolecular capsule held together by four hydrogen bonds [3]. The measured dissociation forces of the heterodimeric capsule represent the mechanical stability of the supramolecular system and allow a quantitative evaluation of the interaction yielding the kinetic dissociation rate constant $k(\text{off})$, the reaction length $x(\beta)$ and the standard Gibbs free energy ΔG_0 according to the Bell-Kramers model.

[1] M. Janke, Y. Rudzevich, O. Molokanova, T. Metzroth, I. Mey, G. Diezemann, P. E. Marszalek, J. Gauss, V. Böhmer, A. Janshoff, *Nat. Nanotechnol.* 2009, 4, 225-229.

[2] C. Schäfer, R. Eckel, R. Ros, J. Mattay, D. Anselmetti, *J. Am. Chem. Soc.* 2007, 129, 1488-1489.

[3] T. Schröder, T. Geisler, B. Schnatwinkel, D. Anselmetti, J. Mattay, submitted.

CPP 9.9 Mon 16:00 H48

Temperature dependent changes in the mechanism of plastic deformation of Polypropylene — •KONRAD SCHNEIDER and ANDREAS SCHÖNE — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01060 Dresden, Germany

The mechanical behaviour of semi-crystalline polymers is dependent on the mechanical behaviour of the crystalline and the amorphous phase as well as their interaction. All those are temperature dependent. Online-WAXS and -SAXS enables to monitor strain dependent the changes within the different phases during deformation and fracture. For the example of Polypropylene it will be demonstrated how the initial lamellae break down into crystalline blocks which disappear in oriented stands in the case of cold drawing, accompanied by cavitation. At higher temperatures the crystalline blocks remain stable and become arranged between fibrillar crystals.

CPP 9.10 Mon 16:15 H48

Robobeads: towards remote friction measurements at small scales — •STEPHAN HERMINGHAUS¹, ZEINA KHAN¹, AUDREY STEINBERGER¹, and RALF SEEMANN² — ¹MPI für Dynamik und Selbstorganisation, Göttingen — ²Universität des Saarlandes, Fakultät für Physik

We have recently discovered that small adhesive spheres may assemble to form aggregates which perform rapid locomotion on a substrate if an external oscillatory drive field is applied. The concept is demonstrated with sub-millimetric wet spheres on a horizontally vibrated flat plate. Quite strikingly, the aggregates tend to align by themselves such as to extract the maximum energy from the drive field. A theoretical treatment shows that this concept is quite robust and under certain circumstances may be scalable down to the sub-micron range