

CPP 21: POSTER: Dynamics and Diffusion

Time: Wednesday 16:00–18:30

Location: Poster B

CPP 21.1 Wed 16:00 Poster B

A new way of implementing partial slip boundary conditions— ●JENS SMIAŁEK¹, FRIEDERIKE SCHMID¹, and MICHAEL ALLEN² —
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Partial slip boundary conditions determine the flow profile in the micrometer scale of modern separation devices where evidence is found that the famous macroscopic no slip boundary conditions are no longer applicable.

We present a new approach to implement partial slip boundary conditions for the study of flow profiles in Dissipative particle dynamics. An extension of the Langevin equation is used to create a viscous layer that exerts friction on the fluid particles in the vicinity of the boundaries. The method is both applicable for particle-based as well as lattice-based algorithms and can be used to generate shear flows like Couette or Poiseuille flow profiles. Crucial parameter for those boundary conditions are the slip length and the position of the hydrodynamic boundaries. Combinations of the above mentioned flow profiles are used to determine both parameters exactly.

The presented method allows to tune the slip length systematically and an analytic equation for the calculation of the slip length as a function of the model parameters can be given.

CPP 21.2 Wed 16:00 Poster B

²H-NMR-Untersuchungen der modifizierten Defektdynamik in dotiertem Eis — ●DANIEL SCHRAFFT¹, BURKHARD GEIL², MARCO SCHEUERMANN¹ und FLORIAN LÖW¹ — ¹Institut für Festkörperphysik, TU Darmstadt, Hochschulstr. 6, D-64289 Darmstadt — ²Lehrstuhl für Experimentelle Physik III, Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund

In einer früheren Studie¹ wurde mittels ²H-NMR der Mechanismus des Protonentransports in hexagonalem Eis untersucht. Die Resultate belegen einen Zwischengittertransport intakter Wassermoleküle. Aufbauend auf der zitierten Arbeit dient dieser Beitrag nun dazu, den Einfluss zusätzlich eingebrachter ionischer Defekte auf die Zeitskala und den Mechanismus des Protonentransports zu untersuchen. Dazu wird an mit HCl, NH₃ und KOH dotierten Proben Spin-Gitter-Relaxationszeiten, stimulierte Echos und Spektren gemessen.

¹B.Geil et al. Phys. Rev. B 72, 014304 (2005)

CPP 21.3 Wed 16:00 Poster B

Molecular dynamics in a glass-forming liquid crystal as studied by broadband dielectric and thermal spectroscopy — ANA BRÁŠ¹, MADALENA DIONÍSIO¹, HEIKO HUTH², CHRISTOPH SCHICK², and ●ANDREAS SCHOENHALS³ — ¹REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, P-2829-516 Caparica — ²University of Rostock, Department of Physics, Universitätsplatz 3, D-18051 Rostock — ³Federal Institute of Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin

Broadband dielectric (10 mHz to 1GHz) and thermal spectroscopy (1 mHz to 10 kHz) was employed to study the molecular dynamics of the nematic liquid crystalline mixture E7. In agreement with theoretical considerations the dielectric spectra shows two relaxation processes. The process at lower frequencies is due to hindered rotational fluctuations about the short molecular axis (delta-relaxation) of the molecules. The process at higher frequencies is related to librational fluctuations around the long molecular axis (tumbling modes). The temperature dependence of the relaxation rate for the delta-process and the tumbling in the nematic phase obey the empirical Vogel-Fulcher-Tamman behavior which is typical for glass-forming systems. For the first time it was shown that the temperature dependence of the relaxation rates for the delta-process and the tumbling modes is essential different using a derivative technique. The comparison of the dielectric with the thermal data gives the result that the glass transition in this system corresponds to the tumbling mode.

CPP 21.4 Wed 16:00 Poster B

Experimentelle Untersuchung der Dynamik im Tetrahydrofuran-Hydrat-Clathrat mit Hilfe der ²H-NMR — ●ANDRE NOWACZYK, BURKHARD GEIL und ROLAND BÖHMER —

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Hydrat-Clathrate können als Speicher- bzw. Transportmedium niedermolekularer Gase von großem Nutzen sein. Für eine effiziente Ausnutzung dieser Möglichkeiten ist es nötig, die Dynamik, sowohl des durch Wasserstoffbrücken gebundenen H₂O-Gitters, als auch der eingeschlossenen Gastmoleküle zu studieren. Als Modellsystem dient in unserem Fall das besonders stabile Tetrahydrofuran-Hydrat-Clathrat. Durch gezielte Isotopenmarkierungen am Clathrat lassen sich mit der ²H-NMR die Bewegungen von Gitter und Gastmolekül getrennt untersuchen. Dazu werden neben Relaxationsmessungen und eindimensionalen Festkörperspektren auch Messungen von Zwei-Zeiten-Autokorrelationsfunktionen verwendet. Letztere erlauben neben der Bestimmung der Zeitskalen auch Erkenntnisse über die Geometrien der dynamischen Prozesse zu gewinnen.

CPP 21.5 Wed 16:00 Poster B

Dielectric response of polar liquids in narrow slit pores— VLADIMIR FROLTSOV¹ and ●SABINE KLAPP^{1,2} — ¹Stranski-Laboratorium, Technische Universität Berlin, Strasse des 17. Juni 115, 10623 Berlin — ²Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Based on molecular dynamics (MD) simulations and a simple (Stockmayer) model we investigate the static and dynamic dielectric response of polar liquids confined to narrow slit pores. The MD simulations are used to calculate the time-dependent polarization fluctuations along directions parallel and perpendicular to the walls, from which the components of the frequency-dependent dielectric tensor can be derived via linear response theory. Our numerical results reveal that the system's response is strongly anisotropic. The parallel dielectric function, $\epsilon_{\parallel}(\omega)$, has Debye-like character very similar to the corresponding isotropic bulk function, $\epsilon_{\text{bulk}}(\omega)$, at the same chemical potential. Indeed, the main confinement effect on $\epsilon_{\parallel}(\omega)$ consists in a shift towards smaller values relative to the bulk function. On the other hand, in perpendicular direction we observe a characteristic peak in the absorption part of the dielectric function, $\epsilon_{\perp}(\omega)$. This peak is absent in the bulk system and reflects strongly pronounced, damped oscillations in the polarization fluctuations normal to the walls.

V. A. Froltsov and S. H. L. Klapp, J. Chem. Phys. **124**, 134701 (2006).

V. A. Froltsov and S. H. L. Klapp, submitted

CPP 21.6 Wed 16:00 Poster B

Determination of microscopic interaction constants with unprecedented accuracy — ●FELIX LEHMKÜHLER, MICHAEL PAULUS, SIMONE STREIT, and METIN TOLAN — Experimentelle Physik I/DELTA, Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund

The poly(propylene glycol) 4000 (PPG4000) - isobutane interface was studied by x-ray reflectivity measurements. The interface was investigated under different pressures between 1.0 bar and 2.6 bar which is close to the condensation pressure of isobutane at the temperature of 289K. While adsorption of molecular thin films of isobutane is expected for hydrophobic interacting systems like glycerol-isobutane or water-propane, the formation of isobutane films on PPG4000 surface is suppressed by the high miscibility of isobutane and PPG4000. Thus no evidence for the formation of isobutane films was found.

The surface roughness of the substrate was estimated to vary between 0.4 nm at 1 bar nitrogen and 0.8 nm at 2.6 bar isobutane pressure. This is explained by the change of surface tension of the PPG4000-isobutane mixture with isobutane pressure. Ideal solution of isobutane in PPG4000 regarding to Raoult's Law is assumed to describe the measurements. The surface tension is calculated with the capillary waves theory to confirm the ideal solution with theoretical models for surface tension behavior of binary liquid mixtures. The Parachor-method and gradient theory are applied. Furthermore, the gradient theory allows to determine microscopic interaction constants qualitatively and quantitatively.

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CPP 21.7 Wed 16:00 Poster B

Diffusion and spin relaxation in thin excited slices — ●ACHIM

GÄDKE¹ and NIKOLAUS NESTLE^{1,2} — ¹TU Darmstadt, Institut für Festkörperphysik — ²BASF AG Ludwigshafen

NMR experiments involving thin excited slices are of interest both for conventional NMR microimaging and for mechanically detected magnetic resonance. Especially in the latter case, the thickness of the excited slices may be well below 1 μm . In samples containing fast-diffusing liquid components such as water, the diffusive exchange of spin magnetization between such a thin excited slice and its surrounding on the time scale of the NMR experiments plays a major role [1]. Using static field gradients of 170 T/m we investigate the effects of periodic excitation inside thin slices. Vertical positioning of the sample cells at μm precision relative to the magnetic field gradient and flat coil design for optimal signal filling factor are prerequisites to systematic studies. A novel experimental cell adapted to such a coil design will be presented and experimental options for manipulating diffusion and relaxation properties of the walls and the liquid in the cell while retaining the exact positioning with respect to the magnet will be discussed. Both simulation and experimental results on the slice's NMR response under periodic excitation will be presented and consequences for further development in micro-MRI and mechanically detected NMR will be discussed.

[1] A. Gädke, N. Nestle, Diffusion Fundamentals 3 (2005) 38.1 - 38.12

CPP 21.8 Wed 16:00 Poster B

Relaxation and transport properties of the macromolecules in solution: effects of the friction tensors — ●ALEXANDER UVAROV and STEPHAN FRITZSCHE — Institut für Physik, Universität Kassel, D-34132 Kassel, Germany; uvarov@physik.uni-kassel.de

Many problems in bio- and chemical physics involve the transport and relaxation properties of macromolecules which immersed in solution. A few well-known examples refer to the dielectric and nuclear magnetic relaxation as well as to the depolarization of the fluorescence light. During the past decade, therefore, a large number of experiments and molecular dynamic simulations (MDS) have been carried out in order to describe the relaxation properties of the macromolecules.

In the present contribution, we explore the question of how the bead-bead and bead-solvent interaction affects the relaxation processes of macromolecules. The behaviour of the friction tensor parameters [1] are analyzed for N-bead chain and for quite different thermodynamical regimes of the solution. The results from our semi-phenomenological theory are found to compare very well with experiment [2] and MD simulations [3] over a wide range of of macromolecule-solvent mass as well as interaction strength ratios.

[1] A. Uvarov and S. Fritzsche, Phys. Rev. E73, 011111 (2006); Chem. Phys. Lett, 401, 296 (2005); Phys. Rev. Lett. submitted (2006).

[2] B. Chen, E. Sigmund and W. P. Halperin, Phys. Rev. Lett. 96, 145502 (2006).

[3] J. R. Schmidt and J. L. Skinner, J. Phys. Chem. B. 108, 6767 (2004); J. Chem. Phys. 19, 8062 (2003).

CPP 21.9 Wed 16:00 Poster B

Lattice Boltzmann simulation of electroosmotic flow — ●MARCELLO SEGA¹ and CHRISTIAN HOLM^{1,2} — ¹Frankfurt Institute for Advanced Studies, Frankfurt, Germany — ²Max Planck Institute for Polymer Research, Mainz, Germany

We report on simulation of electroosmotic flow in a slit pore by

means of coupled Molecular Dynamics - Lattice Boltzmann techniques. Proper dielectric boundary conditions for the confining media are treated by the use of a recently developed extension of the MMM2D and ELC algorithms for electrostatics. The influence of the dielectric jump and of the charge distribution on the confining plates (uniform vs. discrete) is investigated and compared with theoretical predictions.

CPP 21.10 Wed 16:00 Poster B

Is lithium hydride LiH or LiH_{0.5}? This is just a question of time! — ●TYNO ABDUL-REDAH — Inst. f. Chemie, TU Berlin, Str. d. 17. Juni 135, 10623 Berlin, Germany.

The interactions of the particles in a macroscopic system lead to quantum correlated states in which the particles become invisible. The survival time of these states in condensed matter is generally expected to be very short because of the fast and effective decoherence due to interaction with the remaining environment. However, it is indeed possible to measure their effects if the experimental technique is fast enough, e.g., using neutron Compton scattering (NCS) with scattering times of attoseconds. NCS experiments on various solid compounds like metal hydrogen systems have been done [1]. The effect manifests itself by a strong anomalous decrease of the scattering cross section density. E.g., the ionic hydride lithium hydride appears then as LiH_{0.5} rather than LiH in the subfemtosecond time scale of the experiment [2]. The anomaly varies among others with scattering time and with temperature depending on the chemical bond and the electronic environment of the hydrogen in the particular chemical compound. The effect suggests that that the protons do not scatter individually. New experimental results on solid LiH, LaH_x, NbH_x will be presented. The importance of this effect for chemistry and physics will be outlined.

[1] T. Abdul-Redah, C. A. Chatzidimitriou-Dreismann, E. B. Karlsson, Neutron News 15 (2004) 14.

[2] T. Abdul-Redah and C. A. Chatzidimitriou-Dreismann, Physica B 350 (2004) 1035.

CPP 21.11 Wed 16:00 Poster B

The dielectric properties of ionic liquids — ●JOSHUA SANGORO¹, ANATOLI SERGHEI¹, FRANK BORDUSA², and FRIEDRICH KREMER¹ — ¹Institut für Experimentelle Physik I, Universität Leipzig, Linnestraße 5, 04103, Leipzig, Germany — ²Max-Planck-Forschungsstelle für Enzymologie der Proteinfaltung, Weinbergweg 22, D-06120 Halle (Saale), Germany

Broadband Dielectric Spectroscopy (in the frequency range from 0.01 Hz to 10 MHz) at temperatures varying between 190 K to 330 K is employed to study molecular relaxations and ionic charge transport in ionic liquids. The former are observed at low temperatures (\sim 200 K) with the latter giving rise to pronounced increases in the real part of conductivity and respectively the imaginary part of the complex dielectric function, both quantities have pronounced temperature dependence indicating the thermal activities of the underlying ionic charge transport. A remarkably low threshold of the applied electric field E is found to be at 0.3 V/cm, above which non-linear responses take place. Electrode polarization - usually neglected as an unwanted effect - contributes as well depending on various factors as geometry, concentration and the material of the electrode. The results are discussed with respect to recent and old (Debye-Falkenhagen) theories of ionic conduction.