DY 25: Glasses II (joint session of CPP, DF, DY)

Time: Thursday 9:45–12:30 — Location: H38

DY 25.1 Thu 9:45 H38

Dynamics of soft spheres beyond the hard-sphere limit — ●Michael Schmiedeberg and Andrea J. Liu — University of Pennsylvania, Department of Physics and Astronomy, 209 South 33rd Street, Philadelphia, PA 19104-6396, USA

In the limit of low pressures the dynamics of model glass-forming liquids with finite-ranged repulsive interactions are universal. In that limit, where the product of the pressure and the particle volume is small compared to the interaction energy, soft sphere systems behave as hard spheres, so that the dynamics correspond to those of the hard-sphere glass transition and depend only on the ratio of temperature to the product of pressure and the particle volume. However, at higher pressures relative to the interaction energy, there are deviations from this universal behavior that depend on the inter-particle potential. We consider a bidisperse system consisting of soft spheres that repel each other according to a power law potential δ^α where δ is the particle overlap. By using molecular-dynamics simulations, we determine relaxation times as a function of temperature and pressure. We find that the deviations from hard-sphere behavior can be collapsed onto a single curve that depends on $p^{1/\alpha}$.

DY 25.2 Thu 10:00 H38

Correlation between the Diffusion Dynamics and Vibrational Modes of a Model Glass Former — ●Oliver Rubner and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstr. 30, D-48149 Münster, Germany.

In this work we investigate the vibrational modes from computer simulations on a 65 particle binary Lennard-Jones Mixture (BMLJ65) and compare them with the self diffusion dynamics of the particles. As a measure for the dynamics we use the propensities per particle as obtained from an isoconfigurational ensemble which has been introduced by Harrowell (PRL 93, 135701 (2004))

The diffusion dynamics can also be explained in terms of waiting times of the system in inherent structures or metabasins. We compare these waiting times to the vibrational frequencies of the corresponding inherent structures. From this analysis we present the time dependence of the vibrational frequencies which can give some insight into the underlying potential energy surface on which the motion of the system takes place.

DY 25.3 Thu 10:15 H38

Assessing the predictive power of the Reverse Monte Carlo Method for amorphous systems — ●Christian Robert Müller[1], Michael Schuch[2], and Philipp Maass[2] — [1]Theoretical Physics II, Technische Universität Ilmenau, 98684 Ilmenau, Germany. — [2]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany.

The quality of structural models generated by the Reverse Monte Carlo (RMC) method in a typical application to amorphous systems is investigated. To this end diffraction data from a molecular dynamics (MD) simulation of a lithium silicate glass are calculated and used to generate RMC models with different protocols and starting configurations. This allows us to directly compare structural properties of the RMC models with the original MD structures and hence assess the predictive power of the RMC method. It is found that partial distribution functions and properties on small length scales are well reproduced by the RMC modeling. However, properties in the medium-range order, as, for example, ring size distributions are not well captured. We further show that certain medium-range order features of the RMC models can be a mere consequence of the chosen starting configuration when using commonly applied RMC protocols. Due care therefore has to be exercised when extracting structural features from RMC models in the medium-range order regime and when using corresponding information as a basis for subsequent studies of ion transport properties.

DY 25.4 Thu 10:30 H38

Dielectric noise pattern of the Debye- and α-process in a monohydroxy alcohol — ●Tobias Gamp, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Based on the validity of the fluctuation dissipation theorem, dielectric polarization noise spectroscopy allows to measure the dielectric function of a sample electrically non-driven. 2-Ethyl-1-hexanol is one of the prototypical and widely studied glass-forming liquids showing a Debye-like relaxation and the α-peak, the latter associated with the structural relaxation. Since the Debye process is practically invisible in caloric measurements but prominent in conventional dielectric spectroscopy the question whether it could be caused by the presence of electric fields is debated. We show dielectric noise spectra - both voltage and current power spectral densities - and conventional dielectric spectra. Within our experimental resolution and the validity of the fluctuation dissipation theorem both sets of data are in agreement, indicating that the presence of an external field is not necessary for the occurrence of such a Debye peak.

DY 25.5 Thu 10:45 H38

Glass transition in high dimensions — ●Bernhard Schmid and Rolf Schilling — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

We have studied the glass transition of hard spheres with diameter σ for dimensions $d \to \infty$ in the framework of mode-coupling theory (MCT). Assuming that the direct correlation function equals the Mayer function in the limit of high dimensions, we have solved numerically the MCT equations [1] up to $d = 800$. The numerical results for the critical collective and self nonergodicity parameters $f_c(k; d)$ and $f_c^{(s)}(k; d)$ exhibit no Gaussian k-dependence even for $d = 800$. Instead they can be represented by a master function, which vanishes for $k\sigma > \hat{k}_0 d^{3/2}$ with $\hat{k}_0 \cong 0.15$. Inspired by these results, we were able to prove analytically that $f_c(k; d)$ converges to $f_c^{(s)}(k; d)$ for $k\sigma = O(d)$ and $d \to \infty$ and that the critical packing fraction is given by $\varphi_c(d) \sim d^2 2^{-d}$. The non-Gaussian character of $f_c(k; d)$ and $f_c^{(s)}(k; d)$ implies that the hard sphere glass at $\varphi_c(d)$ is not a harmonic solid, even in the limit of high dimensions.

[1] M. Bayer, J.M. Brader, F. Ebert, M. Fuchs, E. Lange, G. Maret, R. Schilling, M. Sperl and J.P. Wittmer, Phys. Rev. E **76**, 011508 (2007)

DY 25.6 Thu 11:00 H38

Brownian dynamics simulation of extensional shear flow in dense colloidal hard-sphere systems — ●Olaf Herbst[1] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Using a novel algorithm based on on event-driven MD simulations adapted for Brownian dynamics, we examine an extensional flow of colloidal particles with periodic boundary conditions. We study the slow dynamics of dense hard-sphere systems when shear rates are high enough to interfere with the slow (alpha) relaxation time. Characteristic features such as the mean-square displacement as a function of time will be discussed for a variety of system parameters.

DY 25.7 Thu 11:15 H38

The influence of the method of glass preparation and ambient conditions on diffusion of alkaline-earth ions in mixed cation glasses — ●Michael Grofmeier and Hartmut Bracht — Institut für Materialphysik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster

Diffusion of alkaline-earth ions in mixed alkali (A) alkaline-earth (M) glasses of the composition xA2O*(3-x)MO*4SiO2 with 0<x<3 was investigated by means of the radiotracer diffusion technique below the respective glass transition temperatures. Our previous studies reveal a distinct dependence of the diffusion behavior of the alkaline-earth ions on the composition x and type of cations in the glass. Additional experiments on the alkaline-earth ions mobility in sol-gel derived glasses of the same composition were performed in this work in order to determine whether the mixed cation effect in alkali-alkaline-earth silicate glasses also holds for sol-gel derived thin glass films. We found that the diffusion behavior of cations in mixed cation silicate glasses is independent of the way of glass preparation. Further diffusion measurements under reducing atmosphere demonstrate a retarded mobility of the alkaline-earth cations.

DY 25.8 Thu 11:30 H38

Crystallization and structural investigation of Eu-doped fluorozirconate-based glass ceramics. — •Christian Passlick[1], Bernd Ahrens[1,2], Bastian Henke[1,2], Jacqueline A. Johnson[3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA

A series of Eu-doped fluorozirconate-based glass ceramics has been developed for medical and photovoltaic applications. In the first case, the materials can be used as x-ray scintillators or x-ray storage phosphors, in the latter case as down-converting top layers for highly efficient solar cells. The glasses are based on a modified ZBLAN composition, i.e. a mixture of Zr, Ba, La, Al, and Na fluorides. They are additionally doped with chlorine ions to initiate the growth of $BaCl_2$ nanocrystals upon thermal processing. Eu^{2+} ions are incorporated into the nanocrystals during the annealing procedure enabling a strong fluorescence upon ultraviolet or x-ray excitation. The nanocrystal size and structural phase depend significantly on the heating conditions and Eu doping level. X-ray diffraction patterns show a structural phase change of the $BaCl_2$ nanocrystals from hexagonal to orthorhombic as annealing temperatures are increased. DSC experiments were performed to obtain activation energies, thermal stability parameters and information on the crystal growth mechanisms.

DY 25.9   Thu 11:45   H38
Time-resolved optical spectroscopy on Er-doped fluorozirconate-based glasses for efficient up-conversion — •Ulrich Skrzypczak[1], Manuela Miclea[1], Jacqueline A. Johnson[2], and Stefan Schweizer[1,3] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA — [3]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale)

Fluorozirconate(FZ)-based glasses have shown their potential as hosts for rare-earth (RE) ions such as Er, in these glasses REs show emissions that would be quenched in other glasses. Such material systems are of practical interest for photon up-conversion. For photovoltaic applications, the efficiency of bifacial solar cells could be vastly improved by an up-converting back layer. Up-conversion is the sequential absorption of two or more low-energy infrared photons by a RE ion followed by subsequent emission of a visible photon. This process is dependent on the intermediate level lifetime of the RE ion, which is determined by the phonon energies of the host material. Low phonon energy glasses like FZ glasses are thus desirable hosts. The lifetimes of the energy levels involved in the up-conversion process are investigated by time-resolved spectroscopy. Short laser pulses at different wavelengths are used for excitation; the emissions are detected via time-correlated photon counting. The radiative and non-radiative decay processes in Er-doped FZ glasses are analyzed and discussed.

DY 25.10   Thu 12:00   H38
Spectral down-conversion in Sm-doped borate glasses for photovoltaic applications — •Marcel Dyrba[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

Samarium fluorescence in glasses has attracted much attention in the past two decades, in particular for studies on spectral-hole burning, excited state absorption, and laser properties. Here, a class of Sm-doped borate glasses has been developed for photovoltaic applications. The fluorescent glass is placed on top of a solar cell and, in the case of Sm^{3+} doping, converts the incident violet/blue part of the solar spectrum to red light which is more efficiently absorbed by the solar cell. The chemical base composition of borate glasses consists of the network former boron oxide and metal oxides as network modifiers. The spectroscopic properties of Sm^{3+}, in particular the fluorescence efficiency, are significantly influenced by the electron negativity of the network modifier. Some of the glasses are additionally doped with silver oxide. Subsequent heat treatment causes reduction of the doped silver ions and leads to the formation of metallic silver nanoparticles. The effect of the local field enhancement around the Sm^{3+} ions, which is due to surface plasmons from the silver nanoparticles being close by, is investigated.

DY 25.11   Thu 12:15   H38
Raman spectroscopy on barium halide nanoparticles in fluorozirconate-based glasses — •Charlotte Pfau[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

Rare-earth(RE) doped fluorozirconate-based glasses show enhanced fluorescence properties when they are additionally doped with Cl or Br ions, which initiate the growth of $BaCl_2$ or $BaBr_2$ nanocrystals, respectively, upon thermal processing. The REs are incorporated into the nanocrystals during the annealing procedure enabling a strong fluorescence upon excitation. A critical parameter for the fluorescence efficiency is the non-radiative decay process from the excited to the ground state. Non-radiative decay processes are determined by the phonon energies of the host system. Low phonon energy systems such as $BaCl_2$ or $BaBr_2$ are desirable hosts for fluorescent ions. The size and structural phase of the nanocrystals depend significantly on the heating conditions; consequently, a series of chlorine- or bromine-doped fluorozirconate-based glasses were analyzed to determine their phonon energy spectra by Raman spectroscopy. For comparison, the phonon spectra of bulk $BaCl_2$, and $BaBr_2$ were investigated.