DF 7 Gläser I (gemeinsam mit FV DY)

Zeit: Montag 10:00–13:00 Raum: TU A060

Hauptvortrag

DF 7.1 Mo 10:00 TU A060

Domain walls in Ising spin glasses — •Timo Aspelmeier — Institut für Theoretische Physik, Universität Göttingen

Domain walls, i.e. the boundaries of energetically low-lying droplets of overturned spins, are at the heart of the droplet theory of spin glasses. They are, however, not limited to droplet theory and their effects can also be found in the rivalling replica field theory (RFT). In particular it is possible to calculate the domain wall exponent θ within RFT exactly. The result of this calculation differs markedly from droplet picture expectations. Numerical measurement of θ can therefore provide a new test to distinguish between the two theories.

DF 7.2 Mo 10:30 TU A060

Atomic Dynamics in Molecular Dynamics Simulations of Glassy CuTi Thin Films — •Sebastian Vauth and S.G. Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We present results on atomic dynamics in metallic glass thin films below the glass transition temperature using molecular dynamics simulations. Thin CuTi films of different compositions are prepared by quenching the liquid to an amorphous state. The atomic dynamics on the amorphous surface and inside the bulk of the samples are quantitatively compared by calculating diffusion constants and jump length distributions. We focus on the collective or single particle character of the diffusion mechanism in dependence of the atom type. In addition, single atom exemplifications are analyzed for the different kinds of atomic dynamics. We find that Cu surface atoms diffuse with a single atom jump dynamics, whereas inside the bulk collective behavior dominates for both species. Our investigations are extended to ion irradiation of the surface with an energy of some keV or less. This work is financially supported by the DFG Sonderforschungsbereich 602, TP B3.

DF 7.3 Mo 10:45 TU A060

Atomic structure and dynamics of alumina melt: A computer simulation study — •Sandro Jahn[1] and Paul A. Madden[2] — [1]GeoForschungsZentrum Potsdam, Sektion 4.1, Telegrafenberg, 14473 Potsdam — [2]PTCL, University of Oxford, South Parks Road, Oxford OX1 3QZ, UK

The construction of accurate and transferable interatomic potentials for oxides and silicates is still a challenging task. The problem is related to the complex electronic structure that is profoundly affected by the interactions of neighboring ions. Effective interactions represented by pair potentials subsume many-body effects in some average sense and may work for a restricted set of coordination environments. However, they do not transfer well to other phases with different coordination environment or mixtures. Here we use an advanced ionic potential that allows for ion polarization, compression and aspherical deformation, and that was optimized by fitting to properties obtained from first principles calculations to study the atomic structure and dynamics of alumina melt. We show that the model is able to reproduce a number of experimental results, such as the static structure factor S(Q), the dynamic structure factor S(Q,ω) and the transport properties. Different cation coordination numbers lead to the splitting of the first peak of the Al-Al radial distribution function which might indicate the dynamic existence of high and low density regions in the melt. Extensions of the current model to multicomponent oxides and silicates will be discussed.

DF 7.4 Mo 11:00 TU A060

Beta-peak dynamics in the hard-sphere colloidal system — •Matthias Sperl — Duke University, Department of Physics, Box 90305, Durham, NC 27708, USA

The nearly-logarithmic decay of the correlation functions found recently in glass-forming *molecular* liquids is identified in the data for the mean-squared displacement of the *colloidal* hard-sphere system at the liquid-glass transition. The solutions of mode-coupling theory (MCT) fit the data well. An asymptotic expansion of the MCT equations of motion explains the nearly-logarithmic decay as a manifestation of the critical relaxation near a simple glass-transition singularity. The later phenomenon is therefore clearly different from the logarithmic decays at higher-order glass-transition singularities. A Cole-Cole formula can be derived rigorously for the nearly-logarithmic relaxation from the leading-order asymptotic expansion. The next-to-leading approximation describes the experimental data for three decades in time.

While previously only known for schematic models, the results identify a beta-peak phenomenon in a microscopic MCT calculation and clarify the origin of this feature of glassy dynamics.

DF 7.5 Mo 11:15 TU A060

Computer Simulations of liquid GeO_2 — •Michael Hawlitzky, Jürgen Horbach, and Kurt Binder — Institut für Physik, Universität Mainz, Staudingerweg 7, D-55128 Mainz

We present molecular dynamics computer simulation results for liquid GeO_2 (at temperatures 6100K $\geq$ T $\geq$ 2530K) and compare it with the appropriate results for the homologous substance SiO_2. This has been done by using classical MD (using a model pair potential developed by Oeffner and Elliott) as well as with the Car-Parrinello *ab initio* technique. We show that the structure and dynamics of GeO_2 exhibit similarities but also distinct differences compared to SiO_2.

In particular, we find that GeO_2 as well as SiO_2 displays a so-called fragile-to-strong transition, i.e. transport coefficients such as the diffusion constants show a change from a power-law behaviour as predicted by mode coupling theory (MCT) at high temperatures to an Arrhenius law at low temperatures. However, in GeO_2 the MCT regime is smaller and the activation energy within the the Arrhenius law regime is, in agreement with experiment, smaller than SiO_2.

DF 7.6 Mo 11:30 TU A060

Intermediate range order and transport processes in viscous aluminium silicates: A computer simulation study — •Patrick Pfleiderer, Jürgen Horbach, and Kurt Binder — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

Glassforming mixtures of SiO_2 with Al_2O_3 with different compositions are investigated by molecular dynamics (MD) computer simulations. These systems form tetrahedral network structures, i.e. both Al and Si are four-fold coordinated by oxygens. We show that these systems exhibit intermediate range order (IRO) that is reflected by prepeaks in partial static structure factors around 0.5 Å^{-1}. The underlying structure is a microphase-separated system where Al-O-rich regions form a percolating network through the Si-O structure. We study how the latter IRO is reflected in dynamical quantities such as the Debye-Waller factor and wave-vector dependent relaxation times.In the temperature range under investigation, i.e. for $T > 2000$ K, structural relaxation can be well described by mode coupling theory.

DF 7.7 Mo 11:45 TU A060

Structure and transport in amorphous alkali silicates: Computer simulation studies — •Jürgen Horbach, Hans Knoth, and Kurt Binder — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

Mixtures of SiO_2 with an alkali oxide such as Na_2O, Li_2O or K_2O are ion-conducting materials for which the mobility of the alkali ions is much higher than that of silicon and oxygen atoms. We present molecular dynamics simulations for different alkali silicates with an alkali oxide content of about 33 mol%. In combination with inelastic neutron scattering [1] we show in the case of sodium disilicate the existence of a network of diffusion channels for the mobile sodium ions that are reflected by a prepeak in the static structure factor around 0.9 Å^{-1}. In systems with two alkali components (namely Li_2O and K_2O) the mixed alkali effect is seen which is most pronounced at low temperatures where the Si-O matrix is not in equilibrium anymore. We find the formation of two subnetworks of diffusion channels for each alkali component, and we discuss how aging effects in the Si-O matrix affect the diffusion of the alkali ions.

[1] A. Meyer, J. Horbach, W. Kob, F. Kargl, and H. Schober, Phys. Rev. Lett. **93**, 027801 (2004).

DF 7.8 Mo 12:00 TU A060

Is there a connection between microscopic particle arrangements and local heterogeneous dynamics in supercooled liquids? — •Hans König — Johannes Gutenberg-Universität Mainz, Institut für Physik, D-55099 Mainz

A binary 2D glass former of superparamagnetic colloids is experimentally investigated. The particles are confined to a plane water-air interface of hanging droplet geometry due to gravity. The particle positions are time-dependently distinguished by video-microscopy. An external magnetic field perpendicular to the monolayer allowed tuning the repulsive dipole-interaction between the induced magnetic moments from outside. The system is described by an interaction parameter Γ, given by the magnetic potential divided by k_BT. Because of this ratio, Γ corresponds to an inverse system temperature.

The amorphous particle configurations are microscopically characterized by triangles of nearest neighbouring particles (TNNP). These triangles form the cages around each particle. Their stability is responsible for locally resolved heterogeneous dynamics and α-relaxations. The local packing is compared to the idealized local density optimized so-called elementary triangles (ET). Large deviations between TNNP and ET detect less densely packed regions in the monolayer. There, fast moving particles are expected. However, does local structure rules dynamics like mode coupling theory predicts?

DF 7.9 Mo 12:15 TU A060

Konnektivität von α- und β-Relaxation in Glasbildnern — •Andre Nowaczyk[1,2], Manfred Winterlich[1,2], Gregor Diezemann[3], Gerald Hinze[3] und Roland Böhmer[1,2] — [1]Experimentelle Physik III, Universität Dortmund, 44221 Dortmund, Germany — [2]Interdisziplinäres Zentrum für magnetische Resonanz, Universität Dortmund, 44221 Dortmund, Germany — [3]Institut für Physikalische Chemie, Johannes Gutenberg-Universität, 55099 Mainz, Germany

Ungeordnete Materialien zeigen neben der strukturellen Relaxation meist auch einen sekundären Prozess vom Johari-Goldstein-Typ. In der Nähe des kalorimetrischen Glasüberganges sind die typischen Relaxationszeiten der beiden Prozesse um mehrere Größenordnungen getrennt. Deshalb liegt die Vermutung nahe, dass α- und langsame β-Relaxation unabhängige Prozesse darstellen. Um diese Vermutung zu testen, untersuchen wir unterkühlte Flüssigkeiten und ungeordnete Kristalle, die sich in der relativen Stärke ihrer β-Relaxation unterscheiden. Als Messmethode setzen wir die im ms...s-Bereich empfindliche stimulierte Echo-Spektroskopie in Kombination mit einem Spin-Gitter-Relaxationsfilter ein. Dies gestattet eine experimentell einstellbare Wichtung der langsamen Echozerfälle durch Relaxationsbeiträge im ms...ns-Bereich. Durch Vergleich der experimentellen Daten mit einem einfachen Modell diskutieren wir, inwieweit eine Selektion nach sekundären Eigenschaften das Erscheinungsbild der Primärrelaxation beeinflusst.

DF 7.10 Mo 12:30 TU A060

Low temperature dielectric properties of molecular glasses — •Catalin Gainaru[1], A. Rivera[1], E.A. Rössler[1], and G. Eska[2] — [1]Physikalisches Institut Experimentalphysik II, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physikalisches Institut Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

We present a systematic study of the dielectric response of simple molecular glass formers below the glass transition temperature T_g down to 4K. The investigations were carried out by applying the new Andeen Hagerling ultra-precision capacitance bridge (resolution $\tan\delta \sim 10^{-6}$, 50Hz - 20kHz). For systems showing no secondary relaxation peak ("type A") a nearly constant loss with an exponential temperature dependence prevails below T_g while for the other systems ("type B") the fluctuations are dominated by the β-process. Though the dynamics can be well distinguished between "type A"and "type B"systems down to 50 - 70 K, below the classification becomes meaningless: for all the investigated systems a crossover to another relaxation phenomena is found. For some systems the dynamics can be described by thermally activated transitions in asymmetric double well potentials. For others this model does not apply. Nevertheless, at temperatures below 10 K, an universal weak frequency dependence similar to the one for inorganic glasses is found for all the systems indicative of the tunneling regime.

DF 7.11 Mo 12:45 TU A060

Molecular reorientation dynamics of a supercooled molecular liquid, ionic liquid, and liquid crystal: a comparison — •Alexander Brodin, Alexei Pugachev, and Ernst Rössler — LS Experimentalphysik II, Universität Bayreuth

We report on a comparative depolarized light scattering study of three rather different supercooled systems: glycerol (molecular liquid), LiCl:5H_2O (ionic liquid) and 5CB (nematic liquid crystal), at temperatures that cover the range from a deeply supercooled glassy state to a high temperature equilibrium liquid state, including the isotropic and supercooled nematic phases of 5CB. In molecular systems composed of anisotropic molecules, the main contribution to the depolarized light scattering comes from molecular reorientations - unrestricted and isotropic in the case of an isotropic liquid (glycerol, H_2O), and restricted about the director in the case of a liquid crystal (5CB). Despite the different nature of the studied systems, they all exhibit qualitatively similar spectra and temperature evolution thereof.