

## DY 8: Glasses I (joint session DY/DF)

Time: Tuesday 10:00–12:40

Location: WIL B321

DY 8.1 Tue 10:00 WIL B321

**Upconversion in fluorozirconate based glass ceramics for high efficiency solar cells** — ●BERND AHRENS<sup>1,2</sup>, BASTIAN HENKE<sup>2</sup>, PAUL T. MICLEA<sup>2,3</sup>, and STEFAN SCHWEIZER<sup>2,3</sup> — <sup>1</sup>Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — <sup>2</sup>Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany — <sup>3</sup>Institute of Physics, Martin-Luther-University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany

Solar cells are unable to use the whole solar spectrum. In particular, sub bandgap photons cannot be absorbed. Materials, which convert in an upconversion process two or more sub bandgap photons into photons with an energy higher than the bandgap energy, are of great interest. Low-phonon energy glasses like fluorozirconate (FZ) glasses are desirable hosts for rare-earth ions such as Er, Ho, Nd, Pr, and Tm because they enable upconverted fluorescence that would be quenched in high-phonon energy glasses. FZ glasses additionally doped with trivalent neodymium and chlorine ions and subsequently annealed show enhanced upconverted fluorescence intensities compared to the as-made samples. The samples were annealed at temperatures up to 290°C to initiate the growth of BaCl<sub>2</sub> nanocrystals therein; the Nd<sup>3+</sup> ion is incorporated in the glass as well as in the nanoparticles. The diameters of the nanocrystals are in the range from a few to several tens of nanometers. The development of glass ceramics doped with Er<sup>3+</sup>, whose optical properties make it a better choice for the application as an upconversion layer on silicon solar cells, is in progress.

DY 8.2 Tue 10:20 WIL B321

**Fluorescence efficiency of samarium-doped glasses and glass ceramics** — ●MARCEL DYRBA<sup>1</sup>, BERND AHRENS<sup>2,3</sup>, PAUL T. MICLEA<sup>1,3</sup>, and STEFAN SCHWEIZER<sup>1,3</sup> — <sup>1</sup>Institute of Physics, Martin-Luther-University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany — <sup>2</sup>Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — <sup>3</sup>Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany

Optically active glasses and glass ceramics offer a broad range of applications; the functionality can be modified by appropriate doping and thermal processing performed after the glass production. Fluorescence from samarium 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. Samarium can enter the glass matrix either in its divalent form and/or as a trivalent ion.

The most efficient fluorescent glasses are characterized by low-phonon energies, a critical parameter leading to reduced non-radiative losses and thus to increased fluorescence efficiencies. However, the phonon frequency is not only dependent on the composition of the matrix the optically-active ion is incorporated into but also by the size of the matrix; in rare-earth doped nanocrystals an increased fluorescence efficiency is found. In this work, we compare the fluorescence efficiency of Sm<sup>2+</sup>/Sm<sup>3+</sup> in different glass systems such as borate glasses, fluorozirconate glasses, or oxyfluoride glasses.

DY 8.3 Tue 10:40 WIL B321

**Improving up-conversion efficiency of rare earth ions by metallic nanoparticles** — ●STEFAN WACKEROW<sup>1</sup>, MARCEL DYRBA<sup>1</sup>, STEFAN SCHWEIZER<sup>1,2</sup>, GERHARD SEIFERT<sup>1</sup>, and HEINRICH GRAENER<sup>1</sup> — <sup>1</sup>Martin Luther university Halle-Wittenberg, 06120 Halle (Saale), Germany — <sup>2</sup>Fraunhofer Center for Silicon Photovoltaics, 06120 Halle (Saale), Germany

A potential way to increase silicon solar cell efficiency is frequency up-conversion of infrared sunlight which can be done by rare earth ions. A novel approach to enhance the up to now rather low up-conversion rates of rare earth ions in glasses is the inclusion of metallic nanoparticles in the glass. The nanoparticles may increase up-conversion efficiencies by the local near-field enhancement and interaction of the plasmon polaritons with rare earth energy levels.

We are therefore studying the co-doping of glasses with rare earth ions and metallic nanoparticles. Generation of silver nanoparticles in glasses is a two-step process. First, silver ions are brought into the glass by field-assisted ion exchange. Second, these glasses are heated in an hydrogen atmosphere, reducing the silver ions to atoms, which

then form silver nanoparticles. This nanoparticle formation has been investigated in commercial rare-earth laser glasses, borate glasses and standard soda lime glass. In order to tune the resonance between plasmon polaritons and the rare earth energy levels, we also modified the nanoparticle shapes from spherical to ellipsoidal by irradiating the samples with intense femtosecond laser pulses.

All modified samples were analyzed by fluorescence measurements.

DY 8.4 Tue 11:00 WIL B321

**Correlation analysis of dielectric polarization noise in glass formers** — ●JENS SCHINDELE, ANDREAS REISER, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

The analysis of dielectric polarization noise is a powerful tool to investigate relaxation processes in dielectric or ionic fluids, glass-forming liquids or glasses. To determine the polarization noise, we measure voltage fluctuations between electrodes immersed in the sample. We show time series analyses of voltage fluctuations of typical glass formers in the temperature range between room temperature and the glass transition temperature. Correlations in space and time probed by a three electrode setup. This enables us to follow the random walk of an effective polarization vector in two dimensions.

DY 8.5 Tue 11:20 WIL B321

**Investigation of the microscopic nature of tunnelling systems in glassy glycerol by using nuclear moments as local probes** — ●MASOOMEH BAZRAFESHAN, CELINE RÜDIGER, GUDRUN FICKENSCHER, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Germany

At low temperatures many properties of glassy materials can be described in the framework of the standard tunnelling model. It assumes the presence of 2-level systems with a broad distribution of energy splittings  $E$ , which arise from particles of mass  $m$  tunnelling between the wells of a double well potential. Up to today, the microscopic nature of these tunnelling systems, i.e. of the tunnelling particles and the tunnelling motion, is not known. We show that nuclear moments on the tunnelling particle can be used as a probe for the microscopic motion of tunnelling systems. We have performed dielectric polarization echo experiments on a series of partially deuterated glycerol samples. The electric quadrupole moments of the deuterium nuclei interacting with local electric field gradients cause a fine splitting of the tunnelling levels, which leads to a quantum beating in small magnetic fields and a pronounced magnetic field dependence of the echo amplitude. The anisotropic interaction of the magnetic dipole moments of the hydrogen nuclei yields a similar effect on a smaller energy scale. By comparing the data to detailed numerical model calculations we were able to extract an effective tunnelling angle and can draw preliminary conclusions about the microscopic properties of the tunnelling entities.

DY 8.6 Tue 11:40 WIL B321

**Mechanisms of atom dynamics on the microsecond scale during the alpha-decay in MD simulated glass forming Ni<sub>0.5</sub>Zr<sub>0.5</sub>** — ●HELMAR TEICHLER — Institut für Materialphysik, Universität Göttingen, Göttingen, Germany

In glass forming melts near TG, the alpha-decay reflects relaxation processes on meso- and macroscopic time scales. Its microscopic explanation is a challenging open question, as it needs to understand emergence of extreme slow dynamics, more than ten orders of magnitude below atomic vibrations, from the atomic motions in the melt. Here we present molecular dynamics simulation results on the microsecond scale for glass forming Ni<sub>0.5</sub>Zr<sub>0.5</sub> at 785 K, aimed at elucidating the microscopic processes of meso-scale dynamics during the alpha-decay well below the critical temperature T<sub>c</sub> of mode coupling theory. From the self intermediate scattering function we find that avalanches of collectively moving atoms, local in space and time, dominate these dynamics. The avalanches are known as higher organized cooperative processes in high-viscous dynamics [H. Teichler, PRE 71, 031505 (2005); JNCS 312, 533 (2002)], and more recently as "democratic particle motion" [G.A. Appignanesi et al. PRL 96, 057801 (2006)]. From our MD data, avalanches turn out as rare events, being created at or near a preceding one with about microsecond delay. Our results are discussed with regard to the dynamical facilitation model of Garrahan

and Chandler.

DY 8.7 Tue 12:00 WIL B321

**Length scale effects in amorphous metals investigated by mechanical loss spectroscopy** — ●DENNIS BEDORF, MORITZ SCHWABE, and KONRAD SAMWER — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Glassy behavior is, in a common assumption, affected by inhomogeneities in internal dynamics. Recent computer studies using molecular dynamics have revealed dynamical heterogeneities on an atomic length scale (Teichler et al., Zink, Mayr[1] and Neudecker). During a shear process shear transformation zones with a radius of about 1.5 nm and string like fluctuations with several nm length occur. Both processes are supposed to be surrounded by an Eshelby-Stress-Field to memorize configuration via the elastic energy [2].

Mechanical spectroscopy using double-paddle-oscillator technique enables us to study mechanical loss in thin films. For this study we choose glassy PdCuSi. The dependence of the loss on temperature and film thickness delivers the activation of certain processes in particular  $\alpha$ - and  $\beta$ - process (wing). Our measurements show a disappearance of the  $\beta$ - process below 50 nm. We discuss this finding in terms of stress fields competing with spatial confinement and surface annihilation.

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[1] M. Zink, K. Samwer, W. L. Johnson and S. G. Mayr, Phys. Rev. B 73, 172203, (2006).

[2] J. S. Harmon, M. D. Demetriou, W. L. Johnson and K. Samwer, Phys. Rev. Lett. 99, 135502, (2007).

DY 8.8 Tue 12:20 WIL B321

**Influence of surfaces on dynamics in polymer thin films - a molecular dynamics study** — ●CHRISTIAN VREE and STEFAN GEORG MAYR — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The influence of free surfaces on the mobility of model polymer chains is investigated with the help of classical molecular dynamics simulations. Below a critical temperature,  $T^*$ , a strong enhancement of the mobility of chains near the surfaces is observed, as calculated from the center-of-mass displacements of the chains. This effect diminishes with increasing temperature. A similar behavior is observed in fluctuations of the radius of gyration, corresponding to conformation changes and hence to structural relaxations. Here the difference between surface and bulk decreases with increasing temperature as well as with increasing time. The temporal evolution of these fluctuations give rise to characteristic sampling times and, thus, activation energies of relaxations of the system. The activation energy for surface relaxations is found to be lower than for bulk relaxations and additionally less temperature dependent.

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[1] C. Vree and S.G. Mayr, submitted to New Journal of Physics (2008)