DF 16: Glasses (Joint Session with CPP and CY)

Time: Wednesday 11:45–12:45 Location: WIL B321

DF 16.1 Wed 11:45 WIL B321

Two-level tunneling systems in amorphous alumina — Alejandro P. Paz[1], •Irina V. Lebedeva[1], Ilya V. Tokatly[1,2], and Angel Rubio[1,3,4] — [1]Nano-bio Spectroscopy Group, Universidad del Pais Vasco, San Sebastian, Spain — [2]IKERBASQUE, Bilbao, Spain — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]European Theoretical Spectroscopy Facility

The decades of research on thermal properties of amorphous solids at temperatures below 1 K suggest that their anomalous behaviour can be related to quantum mechanical tunneling of atoms between two nearly equivalent states that can be described as a two-level system (TLS) [1]. This theory is also supported by recent studies on microwave spectroscopy of superconducting qubits [1]. However, the microscopic nature of TLSs remains unknown. To identify bistable structural motifs in amorphous alumina we have performed extensive classical molecular dynamics simulations. Several motifs with only one or two atoms jumping by considerable distance ~ 0.5 Å were found at temperature 25 K. Accounting for the surrounding environment relaxation was shown to be important up to distances ~ 7 Å. The energy asymmetry and barrier for the detected motifs lied in the ranges 0.5 - 2 meV and 4 - 15 meV, respectively, while their density was about 1 motif per 10000 atoms. Tuning of motif asymmetry by strain was demonstrated with the coupling coefficient below 1 eV. The tunnel splitting for the symmetrized motifs was estimated on the order of 0.1 meV. The properties of the discovered motifs are in good agreement with the available experimental data. [1] G. J. Grabovskij et al. Science 338, 232 (2012).

DF 16.2 Wed 12:05 WIL B321

Resistive Properties of Lithium-Ion Conducting LiSICon Glass Ceramics in Contact with Lithium Metal and Nonaqueous Electrolytes — •Kim Oliver Hofmann[1,2], Meike Schneider[2], Maria-Louisa Reich[2], Miriam Kunze[2], and Michael Vogel[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt — [2]Schott AG Mainz

Lithium-ion conducting glass ceramics with LiSICon type crystalline phase are promising materials as solid electrolytes in future batteries due to their high ionic conductivity, which is higher than $1x10^{-5}$ S/cm. These materials can not only be applied to solid state lithium batteries but also for lithium-sulfur and lithium-air batteries. For these applications the LiSICon materials need to be stable against metallic Li and battery specific liquid electrolytes.

Lithium contact stability is derived by measuring the impedance Z over a period of seven days. In case the glass ceramic reacts with metallic lithium and reduces the polyvalent ions in the glass ceramic like Ge or Ti, the impedance Z is increasing and the sample turns black, noticeably. Further on the impedance spectroscopy is used to determine the interaction of glass ceramics with different liquid electrolytes. The impedance spectra are additionally analyzed by a distribution of relaxation times, based on a distribution function over infinite serial connected RC elements [1]. The resistance contribution of the glass ceramics in contact with liquid electrolytes can be distinguished in interface, grain boundary and grain core resistance by this method.
[1] H. Schichlein et al., J. Appl. Electrochem., 32 (2002) 875- 882

DF 16.3 Wed 12:25 WIL B321

Optical properties of trivalent rare-earth ions in barium borate glasses — •Sebastian Loos[1], Franziska Steudel[2], Bernd Ahrens[1,2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, 06120 Halle (Saale)

Rare-earth doped glasses gain increasing importance in optical devices, such as fibre lasers or light emitting diodes. Luminescence properties of rare-earth ions are well-known, but absolute photoluminescence quantum efficiencies have been insufficiently studied. In this work, series of Sm^{3+}, Eu^{3+}, and Tb^{3+} doped barium borate glasses are investigated for their potential application as frequency down-converters in solid state lighting and photovoltaics. Photoluminescence quantum efficiencies have been analyzed for rare-earth doping levels up to 5 at.%. The best values of more than 50% are achieved for Eu^{3+} doping. To increase the photoluminescence quantum efficiency even further, the Sm^{3+}-doped samples have been co-doped with a second rare-earth ion, namely Eu^{3+} or Tb^{3+}. Here, energy transfer processes between Sm^{3+} and the second rare-earth ion become important; they are discussed in detail.