HL 18: Impurities/amorphous semiconductors

Time: Tuesday 12:00–13:00 Location: POT 151

HL 18.1 Tue 12:00 POT 151

Pulsed electrically detected magnetic resonance study of spin relaxation and recombination in thin-film silicon solar cells — •Matthias Fehr[1], Jan Behrends[1], Alexander Schnegg[1], Klaus Lips[1], Bernd Rech[1], Oleksandr Astakhov[2], and Friedhelm Finger[2] — [1]Helmholtz-Zentrum Berlin, Silizium Photovoltaik, 12489 Berlin, Germany — [2]Forschungszentrum Jülich, IEF-5 Photovoltaik, 52425 Jülich, Germany

We have investigated the influence of paramagnetic states on electronic transport processes in thin-film pin solar cells with pulsed Electrically Detected Magnetic Resonance (pEDMR) at X-Band frequency and low temperature (10 K). The solar cells consist of an intrinsic microcrystalline absorber layer and amorphous or microcrystalline n/p contacting layers. In addition to the identification of the participating paramagnetic centres by their g-factors, pEDMR can be used to study the dynamics of the electronic processes in detail. We present measurements of modified EPR pulse sequences in order to identify the dominating relaxation mechanisms within correlated solid-state spin-pairs. By this technique a monitoring of the spin and charge motion is possible. In the outlook we present measurements of the electron spin echo envelope and critically discuss modulations in terms of dipolar coupling within the spin-pairs or hyperfine couplings to surrounding nuclei.

HL 18.2 Tue 12:15 POT 151

First-principles calculations on self-diffusion in indium oxide — •Péter Ágoston[1], Paul Erhart[2], Andreas Klein[1], and Karsten Albe[1] — [1]Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23 64287 Darmstadt — [2]Lawrence Livermore National Lab, California, USA

Indium oxide/ITO (indium tin oxide) is one of the most commonly used TCO materials (transparent conducting oxide). Although it is well known that point defects govern the materials' functional properties, so far very little is known about their thermodynamic and kinetic properties. Defect concentrations sensitively depend on temperature, oxygen processing gas composition (oxygen partial pressure) and impurity level like the commonly used tin substitutional doping. Thus, different deposition techniques and temperature processing steps directly affect the defect equilibria and consequently the materials properties, which makes a more detailed understanding highly desirable. Therefore, we have conducted extensive calculations based on density functional theory in order to calculate the formation and migration energies of the dominant intrinsic point defects. Additionally, we have derived the entropy contributions to defect formation and migration in a rigorous way. Using this input data we are able to calculate the Fermi energy in the material as a function of temperature, oxygen partial pressure and doping. The defect concentrations at the calculated Fermi energy are then used to predict the diffusivity at different environmental conditions.

HL 18.3 Tue 12:30 POT 151

Structural modification of swift heavy ion irradiated amorphous Ge layers — •Werner Wesch[1], Claudia S. Schnohr[2], Patrick Kluth[2], Zohair S. Hussain[2], Leandro L. Araujo[2], R. Giulian[2], David J. Sprouster[2], Aydan P. Byrne[2], and Mark C. Ridgway[2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Department of Electronic Materials Engineering, Australian National University, Canberra

To study the effect of high electronic energy deposition on amorphous Ge layers, crystalline Ge wafers were amorphised to a thickness of 3.2μm by multiple Ge ion implantation at 80 K. A Au grid was then evaporated on the sample surface which was partly masked during the irradiation. The samples were then irradiated with various fluences of 185 MeV Au ions at room temperature and an angle of incidence of 45° with respect to the surface normal. The irradiated samples were analysed by optical microscopy, surface profilometry and scanning electron microscopy (SEM). Subsequent to irradiation, a change in sample surface colour from light brown to black with increasing ion fluence was readily apparent. The change of colour was accompanied with swelling of the amorphous layer, the latter also increasing with ion fluence. The swelling was a consequence of void formation within the amorphous layer, which transformed into a sponge-like porous structure at higher ion fluences. Additionally, as in a-Si, a surface shift in the irradiated region along the projection of the ion beam to the sample surface increasing with the ion fluence was observed demonstrating liquid polymorphism is common to these two semiconductors.

HL 18.4 Tue 12:45 POT 151

Ab-initio calculations of hyperfine parameters for various Si-dangling bond models — •Gernot Pfanner, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck Institute for Iron Research, Computational Materials Design, Max-Planck-Strasse 1, D-40237 Duesseldorf

Thin-film silicon solar cells are considered as low-cost successors of bulk crystalline Si solar cells. However, at the moment, their efficiency is severely limited by light-induced defects. The nature of the so-called 'Staebler-Wronski' effect, i.e. light-induced metastable changes in the properties of hydrogenated amorphous silicon, is not yet understood and remains challenging. Electron-paramagnetic resonance (EPR) is a key technique to improve our knowledge about the local atomic structure and, consequently, about the processes causing the long-term drop in the conversion rate and thus in the device performance. However, the interpretation of the EPR spectrum requires theoretical insights in the influence of the microscopic structure on the hyperfine parameters, which we provide by first-principle calculations. For this purpose, we employ density-functional theory and a pseudopotential approach, in which the all-electron wave function is reconstructed from a combination of free-atom and pseudo-wavefunctions. Within this approach, we consider various dangling-bond models and study the sensitivity of the hyperfine parameters to structural features in the vicinity of the defect. A comparison with available experimental data allows us to identify realistic dangling bond models.