HL 39: Impurities/amorphous semiconductors

Time: Thursday 12:15–13:00 Location: H14

HL 39.1 Thu 12:15 H14

Defect density profiling by absorption depth dependent thermally stimulated currents in microcrystalline silicon — •Sven Burdorf, Nacera Souffi, Gottfried Bauer, and Rudolf Brüggemann — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg

The defect density profile of an inhomogeneous microcrystalline silicon sample (μc-Si:H) is studied using the experimental technique of thermally stimulated currents (TSC). The TSC measurements are carried out with initial excitation conditions that differ by the absorption depths of the light illuminating the sample. The measured TSC spectra do not change with varying absorption depths. The determination of the densities of gap states leads to the conclusion that the defect density near the surface is at least one order of magnitude larger than the average defect density over the entire sample. In addition, constant photocurrent method (CPM) results support this interpretation.

HL 39.2 Thu 12:30 H14

Influence of doping and codoping on the electronic and optical properties of Si nanocrystallites — •Luis Ramos, Jürgen Furthmüller, and Friedhelm Bechstedt — Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und -optik, Max-Wien-Platz 1 D-07743 Jena, Germany

Quantum confinement in Si nanocrystallites (NCs) leads to interesting optical and electronic properties that can be useful in optoelectronics, photovoltaics, and nanoelectronics. Since doping is a fundamental process in semiconductors, investigations have been performed to establish the doping efficiency in Si NCs in comparison with bulk. Recent experiments confirm that codoping with group-III and group-V can enhance the intensity of luminescence in Si NCs by preventing radiationless Auger recombinations, which are the main problem in shallow-impurity doping in Si NCs. Experiments usually refer to an ensemble of Si NCs with a size and shape distribution, what can make the interpretation of the results more difficult. On the other hand, theoretical methods can be used to investigate the electronic properties and optical transitions of a single Si NC.[1] We perform ab initio calculations for doped and codoped Si NCs, which are based on density-functional theory and generalized-gradient approximation to study their electronic and optical properties. The formation energy of the impurities, electronic structure and optical spectra, and radiative lifetimes for doped and codoped Si NCs are discussed.[1] L.E. Ramos, J. Furthmüller, and F. Bechstedt, Appl. Phys. Lett. **87**, 143113 (2005); Phys. Rev. B **72**, 045351 (2005); Phys. Rev. B **70**, 033311 (2004).

HL 39.3 Thu 12:45 H14

Non-periodicity in atomic structure of cadmium sulfide CdS nanoparticles — •Andrey Vorokh[1,2], Andrej A. Rempel[1,2], and Andreas Magerl[2] — [1]Institute of Solid State Chemistry, Russian Academy of Sciences, Pervomaiskaya 91, GSP-145, Ekaterinburg 620219, Russia — [2]Crystallography and Structural Physics, University of Erlangen-Nuremberg, Staudtstrasse 3, 91058 Erlangen, Germany

By means of X-ray diffraction experiment and ab initio calculation of powder diffraction intensity using Debye equation it is shown that the atomic structure of cadmium sulfide (CdS) nanoparticles prepared by wet chemical method is disordered. The disordered atomic structure is a closed packed atomic structure with the tetrahedral coordination for both elements, cadmium and sulfur, but with a non-periodical sequence of the closed-packed planes types A, B, and C. The free energy of the disordered structure is higher in compare with the energy of known for CdS crystalline structures, wurtzite (B4 type, ABABAB. . . sequence of closed-packed planes) and zincblende (B3 type, ABCABC. . . sequence of closed-packed planes).