HL 87: Goup IV elements and their compounds II

Time: Thursday 15:45–17:30 Location: H15

HL 87.1 Thu 15:45 H15

Indirect to direct gap transition in strained and unstrained group-IV semiconductor alloys — Christian Eckhardt, •Kerstin Hummer, and Georg Kresse — University of Vienna, Computational Materials Physics, Sensengasse 8/12, 1090 Vienna, Austria

The basic problem of the well established Si technology is the indirect nature of the fundamental band gap of the elemental group-IV semiconductors resulting in inefficient light absorption and emission. To overcome these limitations, advanced (opto)electronic device design concentrates on strategies to transform materials consisting of group-IV elements from indirect into direct gap semiconductors. One promising route established is the introduction of strain either by alloying or by growing heterostructures/superlattices. Besides the extensively investigated Si/Ge system, the Sn_xGe_{1-x} alloy turned out to be very promising [1].

In this work, we focus on Sn_xGe_{1-x} and C_xGe_{1-x} random substitutional alloys. The transition from an indirect to a direct gap semiconductor in strained and unstrained alloys as a function of the Sn/C content between $0 \leq x \leq 0.5$ is investigated within density functional theory by means of both, a supercell approach and the Virtual Crystal Approximation. Accurate band structures are obtained with the modified Becke-Johnson exchange potential in combination with LDA correlation [2].

[1] H. Lin et al., Appl. Phys. Lett. **100**, 102109 (2012)
[2] F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009)

HL 87.2 Thu 16:00 H15

Defect states at c-Si/a-$Si_3N_xH_y$ interfaces — •Leif Eric Hintzsche[1], Gerald Jordan[1], Martijn Marsman[1], Machteld Lamers[2], Arthur Weeber[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]ECN Solar Energy, P.O. Box 1, 1755 ZG Petten, Netherlands

Amorphous silicon nitrides are deposited on crystalline silicon as antireflection and passivating coatings. Up to date detailed knowledge about the interfaces is largely lacking. We have investigated the electronic and structural properties of c-Si/a-$Si_3N_xH_y$ interfaces obtained by large scale ab initio molecular dynamics simulations. Over 500 independent samples have been generated for each considered stoichiometry to perform a reliable defect analysis. While the classes of dominant defect states coincided with previous bulk calculations, we found a considerably increased defect density at the interface. By applying an energy and spatially resolved defect analysis, we observed that most of the defect states originate from the first silicon nitride layer at the interface. Additionally, we examined passivation effects of hydrogen at the interface which play an important role to increase the efficiency of modern solar cells.

HL 87.3 Thu 16:15 H15

First stages of 4H-SiC crystal growth: *ab initio study* — •Elwira Wachowicz[1,2] and Adam Kiejna[1] — [1]Institute of Experimental Physics, University of Wroclaw, Wroclaw, Poland — [2]Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Warsaw, Poland

The wide band-gap semiconductor silicon carbide has attracted a great interest during the past decades because of number of properties which make it very attractive for many applications in electronic devices. For electronic applications purposes hexagonal 4H-SiC is the preferred polytype. One of the main problems in the development of the SiC-based electronics is still poor quality of the SiC crystals. Therefore, it is necessary to understand the interaction of basic building bricks like Si, C, Si_2C and SiC_2 with the surface. Since hexagonal SiC crystals grow along <0001> direction the interaction of Si, C and Si_2C interaction with Si- and C-terminated {0001} surfaces is examined within DFT framework. The most favourable adsorption sites are identified. Qualitative *ab initio* molecular dynamic simulations show that molecules bind to both examined surfaces without dissociation. It is confirmed by quantitative DFT studies showing that there is no barrier for the molecule adsorption. Moreover, a possible mechanism of Si_2C on-surface dissociation is examined.

HL 87.4 Thu 16:30 H15

Reactive Ion Etching of Nano- and Ultrananocrystalline Diamond Films for Fabrication of Nanopillars — Christo Petkov, Emil Petkov, Florian Schnabel, Wilhelm Kulisch, Johann Peter Reithmaier, and •Cyril Popov — Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

One-dimensional diamond nanostructures, namely diamond nanopillars, have been prepared using nano- and ultrananocrystalline diamond films (NCD and UNCD, respectively) as starting materials. The fabrication process of arrays of nanopillars with diameters from 200 nm to 1000 nm consisted of their definition by electron beam lithography (EBL) applying gold or silica as a hard mask and subsequent inductively coupled plasma reactive ion etching (ICP-RIE) with oxygen. The major ICP-RIE parameters, like ICP power, RF power, working pressure, oxygen flow, etc. were optimized with respect to the quality of the nanopillars and the etching rate, which was monitored in situ with an interferometer. Furthermore, the influence of the hard mask material and pillar diameter on the geometry of the nanostructures was studied. The fabricated diamond nanopillars, especially those from NCD, can be used as photonic devices for integration of NV centers during the film growth or by follow-up ion implantation.

HL 87.5 Thu 16:45 H15

Dephasing in Ge/SiGe quantum wells measured by means of coherent oscillations — •Kolja Kolata[1], Niko S. Köster[1], Alexey Chernikov[1], Michael J. Drexler[1], Eleonora Gatti[2], Stefano Cecchi[3], Daniel Chrastina[3], Giovanni Isella[3], Mario Guzzi[2], and Sangam Chatterjee[1] — [1]Philipps-Universität Marburg — [2]L-NESS, Università di Milano Bicocca — [3]L-NESS, Polo di Como

In general, all coherent effects in optically excited materials depend crucially on the dephasing of the addressed states. Therefore, knowing the duration of the coherence and understanding the dephasing mechanisms is mandatory in order to interpret coherent effects correctly. Dephasing mechanisms are often summarized in the dephasing time which is also used as a phenomenological damping parameter in theoretical descriptions. Ge/SiGe heterostructures as a material system are especially interesting for dephasing studies since they exhibit strong nonlinear coherent responses such as the giant dynamical Stark effect. We present a dephasing time analysis of the three lowest excitonic resonances in Ge/SiGe quantum well samples for the temperatures down to 7K by coherent oscillations spectroscopy (COS). The results are compared to the line widths of the excitonic resonances determined by linear absorption measurements. Strikingly, the lowest direct-gap transition in the best quality sample is dominated by homogeneous broadening over the entire investigated temperature range. This is explained by the fast inter-valley scattering of the electrons which leads to intrinsically short dephasing times of merely 300 fs as an upper limit.

HL 87.6 Thu 17:00 H15

Photonic crystal microcavities for the luminescence enhancement of Si/Ge-Quantum dots around 1550nm wavelength — •Viktoriia Rutckaia[1], Benjamin Koehler[1], Vadim Talalaev[2], Frank Heyroth[3], and Joerg Schilling[2] — [1]Martin-Luther University, Halle (Saale), Germany — [2]Centre for Innovation Competence SiLi-nano, Halle (Saale), Germany — [3]Interdisciplinary Center of Materials Science, Halle (Saale), Germany

Defects in two dimensional photonic crystal slabs represent microcavities with small mode volumes and can exhibit large Q-factors. This can lead to a large enhancement of spontaneous emission rate causing an overall enhancement of radiative recombination efficiency. This was also already observed for the photoluminescence of Ge quantum dots in Si [1]. The aim of this work is to show how the Q-factor of certain defect modes can be altered by adjusting the geometry of the pores adjacent to the cavity. This involves changing their diameter and variation of their positions. We present band gap and defect resonance calculations for 2D photonic crystal cavities using MIT mpb program [2], and COMSOL multiphysics. From the field distribution the mode volume is determined and theoretically possible Purcell factors are obtained. Experimental studies of the luminescence enhancements in

the micro cavities involve micro-photoluminescence measurements on Ge quantum dots embedded in Si. Defect resonances are observed and their Q-factors were obtained from the luminescence spectra. [1] J.S.Xia,Y.Ikegami, and Y.Shiraki, Appl.Phys.Let.89,201102(2006),[2] Steven G.Johnson and J.D.Joannopoulos, Opt.Exp.8,3,173-190(2001)

HL 87.7 Thu 17:15 H15

Side-wall damage analysis of low-k interlayer dielectric from energy-filtered transmission electron microscopy — •Pradeep K. Singh[1], Sven Zimmermann[2], Steffen Schulze[1], Stefan Schulz[2,3], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany — [2]FraunhoferInstitute for Electronic Nano Systems (Fraunhofer ENAS), Dept. BEOL, D-09107 Chemnitz, Germany — [3]Chemnitz University of Technology, Center for Microtechnologies, D-09107 Chemnitz, Germany

The continues shrinkage in device dimensions leads towards the inevitable replacement of the conventional SiO2 material as an inter-layer dielectric with lower dielectric constant (low-k) material. Several low-k dielectric materials were developed for this purpose. Among these, the organosilicate glasses are of preferred choice due to their excellent properties as an inter-layer dielectric. The organosilicate glasses consist of the methyl groups doped inside the SiO2 networks. One of the major challenges to incorporate the low-k dielectric materials in device production is the side-wall damage of these materials. The side-wall damage regions were characterized by the energy-filtered transmission electron microscopy. The etch and ash plasma used in the standard processes, damaged the side-walls in the 10th of nano-meter region. The side-walls were found to be depleted from carbon and hence behave more like SiO2 material.Due to the higher dielectric constant of SiO2 as compared to the low-k dielectric materials, the effective dielectric constant of the low-k material increases by the plasma treatment.