

HL 11: Carbon: Nanotubes, Diamond and Silicon Carbide

Time: Monday 11:45–14:00

Location: EW 203

HL 11.1 Mon 11:45 EW 203

Electronic properties of silicon carbide surfaces and interfaces

— ●ANDRE KONOPKA, TIM BAUMGARTEN, SIEGMUND GREULICH-WEBER, EVA RAULS, WOLF GERO SCHMIDT, and UWE GERSTMANN — Physics, University of Paderborn, Paderborn, Germany

Micro- and nanocrystalline materials provide new applications not only because of their potential to shrink devices, but also due to their new electrical and optical properties. Understanding the origin of these properties is essential to design and optimize these materials and the resulting devices. In these systems properties of surfaces and interfaces can dominate that of the bulk. Microcrystalline silicon carbide ($\mu\text{c-SiC}$) have become an attractive new class of advanced microstructured materials for optoelectronic applications due to their wide band gap and advanced chemical and mechanical properties. We use a sol-gel process for growing $\mu\text{c-SiC}$ allowing arbitrary doping. To understand the origin of our experimental results [1,2] we performed theoretical calculations in the framework of density functional theory (DFT). In this work we present the results of different surfaces of SiC. We discuss how the electronic properties of the different surfaces interact with n- and p-type doping of SiC. Based on these calculations we propose a model that explains the charge transfer at an interface between SiC and an organic semiconductor. The calculated surface band structures can also help to understand other experimental results, like conductivity and EPR signatures.

[1] A. Konopka et al (2010) IOP Conf. Ser.: Mater. Sci. Eng. 15 012013, [2] A. Konopka et al (2011). MRS Proceedings, 1322

HL 11.2 Mon 12:00 EW 203

Electrical and Chemical Passivation of 6H-SiC Surfaces by Chlorine Termination — SEBASTIAN SCHOELL, ●MATTHIAS SACHSENHAUSER, JOHN HOWGATE, JOSE GARRIDO, MARTIN BRANDT, MARTIN STUTZMANN, and IAN SHARP — Walter Schottky Institut, Technische Universität München, Garching, Germany

In recent years, growth and processing of SiC has considerably improved. However, practical ways of chemical and electrical passivation of SiC surfaces are still rare. In particular, etching in HF yields hydroxylated surfaces with high defect densities. Here, we utilize plasma processing methods to achieve chlorine-terminated n-type (0001) 6H-SiC surfaces. Static water contact angle and atomic force microscopy show a transition of the wetting behavior from hydrophilic to hydrophobic surfaces following chlorine termination without affecting the surface roughness. Accordingly, X-ray photoelectron spectroscopy reveals an increased chlorine core level intensity together with a significant reduction of oxygen. Chlorine desorption at elevated temperatures of up to 425°C suggests saturation of terminal atoms rather than near surface incorporation of chlorine. The electronic properties of the plasma treated surfaces are examined with contact potential difference and surface photovoltage measurements and show the formation of negative surface dipoles as well as approximately flat band surface potentials, indicative of a successful termination of electrically active surface defect sites. Finally, we demonstrate that the halogenated surfaces enable the formation of functional self-assembled monolayers providing controlled chemical functionalities for bioelectronic and biosensor applications.

HL 11.3 Mon 12:15 EW 203

H and Si interaction with 4H-SiC surfaces — ●ELWIRA WACHOWICZ^{1,2} and ADAM KIEJNA¹ — ¹Institute of Experimental Physics, University of Wrocław, Wrocław, Poland — ²Interdisciplinary Centre for Materials Modeling, Warsaw, Poland

Silicon carbide due to its wide band gap, it is suitable for applications related to high power, high frequencies, and high temperatures. The most commonly precursor for silicon in homoepitaxial VPE-growth of SiC is silane. Therefore, the understanding of the Si and H interaction with SiC surfaces is essential to gain better control over the crystal growth process. In this paper the ab initio calculations of the interaction of Si and H atoms with Si- and C-terminated SiC surfaces are presented. The only stable adsorption site on the stoichiometric 4H-(0001) and (000 $\bar{1}$) surfaces is situated on top of the topmost surface atom for H coverages ranging from 0.11 to 1 monolayer (ML). H atom binds stronger on the (000 $\bar{1}$) with adsorption energy about -6 eV independent of the H coverage. The H adsorption energy on Si-terminated (0001) surface changes from -5.6 eV at 0.11 ML to -5.2 eV at 1 ML.

The changes in the first interlayer distances are linear with respect to the H coverage for both surfaces. The molecular dynamic simulations show dissociative adsorption of H₂ molecule. Consequently, the study of Si adsorption on partially H covered or H saturated surfaces are performed. Those allow to identify the most favourable Si adsorption sites. The influence of the Si and H coadsorption on the atomic and electronic structure of the 4H-SiC(0001) and (000 $\bar{1}$) surfaces is analysed.

HL 11.4 Mon 12:30 EW 203

Towards a quantum point contact on hydrogen-terminated single-crystalline diamond — ●MORITZ HAUF, PATRICK SIMON, MAX SEIFERT, MARKUS STALLHOFER, MARTIN STUTZMANN, ALEXANDER HOLLEITNER, and JOSE A. GARRIDO — Walter Schottky Institut and Zentrum für Nanotechnologie und Nanomaterialien, Am Coulombwall 4, 85748 Garching

The two-dimensional hole gas which forms at the surface of hydrogen-terminated diamond has already been used for the fabrication of in-plane gated field effect transistors in the past. Until now, no quantum effects have been observed in these structures. However, the two-dimensional nature of the hole gas offers a good starting point for the fabrication of lower-dimensional structures, similar to GaN/AlGaN heterostructures.

In this work we use e-beam lithography to selectively oxidize the H-terminated diamond surface in order to create conductive channels with nano-scale dimensions. We show Coulomb-blockade on surface-conductive channels with a width of 100nm. Furthermore, in-plane gate structures are used to approach conductance quantization in this material system at temperatures below 4K. Varying the gate voltage, we observe stepwise changes of the conductance in channels with widths of 100nm, 150nm, 200nm, and a length of 100nm. We discuss the origin of the conductance quantization in terms of the dimensionality of the hole-gas and possible Coulomb blockade effects at the surface of H-terminated diamond.

HL 11.5 Mon 12:45 EW 203

Charge transfer in diamond-based biohybrid systems for energy harvesting applications — ●MICHAEL METZGER, ROBERTA CATERINO, MATTHIAS SACHSENHAUSER, MARTIN STUTZMANN, and JOSE ANTONIO GARRIDO — Walter Schottky Institut, Technische Universität München, Germany

The understanding of charge transfer on the nanometer scale is of fundamental interest for a multitude of applications like molecular electronics, sensing, and catalysis. In addition, the energy conversion processes involved in photosynthesis represent a blueprint for future nanoscaled bioelectronics.

Our research aims at the immobilization of photosynthetic reaction centers (RCs) on diamond substrates for the study of direct charge transfer under photo excitation. For the covalent immobilization of RCs, we will discuss a novel functionalization concept which has been extensively investigated using a variety of redox species. Aminocaproic acid molecules were grafted onto H-terminated boron-doped polycrystalline diamond surfaces in order to introduce functional carboxylic groups which can be used for tethering redox species and biomolecules via covalent amide bonds. Cyclic voltammetry, square wave voltammetry, and electric impedance spectroscopy were employed to characterize the grafting of several molecules and biomolecules such as aminomethyl ferrocene, horseradish peroxidase, and cytochrome c. We have investigated the spectrally resolved photocurrent of RCs immobilized on boron-doped polycrystalline diamond, as well as on gold substrates.

HL 11.6 Mon 13:00 EW 203

Carbon nanotube Fermi energy shifts upon deposition on a substrate revealed by Raman spectroscopy — ●BENJAMIN HATTING¹, SEBASTIAN HEEG¹, FRANK HENNRICH², RALPH KRUPKE², and STEPHANIE REICH¹ — ¹Freie Universität Berlin, Berlin, Germany — ²Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Raman spectroscopy of single-walled carbon nanotubes (SWNTs) reveals a variety of information about the samples under study, such as their composition in terms of chirality and the amount of defects. Additionally, the lower-frequency component of the high-energy modes (HEM) in metallic tubes is sensitive to the position of the Fermi level.

This component arises from longitudinal optical (LO) vibrations. It appears at lowered frequencies of about 1550cm^{-1} when the Fermi energy is at its intrinsic value due to the presence of a Kohn anomaly at the Γ point in the LO phonon branch.[1] We report the observation of a downshift of the metallic LO peak along with a broadening of its width upon deposition of a chirality-enriched tube sample[2] on a Si substrate. We explain our observations in terms of two Fermi energy shifts. The results imply that simple inspection of the HEM lineshape is insufficient to judge the presence of metallic tubes in a sample with an unknown chirality distribution.

HL 11.7 Mon 13:15 EW 203

Two-color pump-probe study of single-walled carbon nanotubes — •OLGA A. DYATLOVA¹, CHRISTOPHER KOEHLER², ERMIN MALIC², JORDI GOMIS-BRESCO¹, JANINA MAULTZSCH³, ANDREY TSAGAN-MANDZHIEV¹, TOBIAS WATERMANN², ANDREAS KNORR², and ULRIKE WOGGON¹ — ¹Institut fuer Optik und Atomare Physik, Technische Universitaet Berlin, 10623 Berlin, Germany — ²Institut fuer Theoretische Physik, Technische Universitaet Berlin, 10623 Berlin, Germany — ³Institut fuer Festkoerperphysik, Technische Universitaet Berlin, 10623 Berlin, Germany

Due to their remarkable properties carbon nanotubes (CNT) have big application potential which is already implemented in some real devices and products. A better understanding of the ultrafast relaxation dynamics of optically excited carriers in single walled carbon nanotubes is of crucial importance for the realization of their application potential. In this work, we perform two-color pump-probe experiments to determine the decay behavior of (8,7), (10,2), (11,3), and (12,1) nanotubes. We find the relaxation dynamics to be characterized by three decay times in ps, tens of ps and few hundreds of ps ranges. Our results are modeled within a microscopic approach based on the density matrix formalism. Our calculations reveal that the component in the range of 5-10 ps is due to the intraband carrier-phonon scattering.

HL 11.8 Mon 13:30 EW 203

Permanent Dipole Moments of Localized Carbon Nanotube Excitons — •JAN GLÜCKERT, MATTHIAS HOFMANN, and ALEXANDER HÖGELE — Fakultät für Physik and Center for Nano Science (CeNS), Ludwig-Maximilians-Universität, München, Germany

Semiconducting single-walled carbon nanotubes exhibit photoluminescence emission in the near infrared due to recombination of excitons [1-3]. Recent observation of photon anti-bunching in the cryogenic

photoluminescence of individual nanotubes suggests that exciton localization at low temperatures dominates the spectral response [4].

We investigate the emission spectra of individual CoMoCat nanotubes as a function of external electric field. We fabricated a sample that allows us to apply static electric fields perpendicular to the nanotube axis and record their spectral response in a confocal microluminescence setup at cryogenic temperatures.

We observe spectral shifts up to several linewidths and a linear dependence of the emission energy on the electric field. We interpret our findings in terms of a linear DC Stark effect due to permanent dipole moments of localized excitons. From the linear slope we deduce values for the exciton dipole moments and find a sub-Angstrom electron-hole separation.

[1] M. J. O'Connell et al., Science 297, 593 (2002).

[2] J. Maultzsch et al., Physical Review B 72, 241402 (2005).

[3] F. Wang et al., Science 308, 838 (2005).

[4] A. Högele et al., Physical Review Letters 100, 217401 (2008).

HL 11.9 Mon 13:45 EW 203

Photoluminescence of pristine carbon nanotubes — •MATTHIAS HOFMANN, JAN GLÜCKERT, and ALEXANDER HÖGELE — Fakultät für Physik and CeNS, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, D-80539 München, Germany

Semiconducting carbon nanotubes are an ideal material for the study of optical phenomena in one-dimensional systems. Recent experiments have shown that nanotubes exhibit the quantum optical effect of strong photon anti-bunching [1]. However, photoluminescence studies also revealed that the intrinsic optical properties of the commonly used material are partly masked due to the surrounding environment and defects in the nanotube crystalline structure.

By means of chemical vapour deposition we fabricated samples with freely suspended pristine carbon nanotubes with diameters in the sub-nanometer range. In contrast to commercial material of same chirality the photoluminescence of our suspended nanotubes reveals suppressed spectral diffusion and emission linewidths below the resolution limit of our spectrometer ($<100\text{ }\mu\text{eV}$). Furthermore, photoluminescence lifetimes of several nanoseconds are no longer limited by rapid quenching - now exceeding previously reported decay times [2] by one order of magnitude in accordance with *ab initio* theory predictions [3].

[1] A. Högele *et al.*, Phys. Rev. Lett. **100**, 217401 (2008)

[2] A. Hagen *et al.*, Phys. Rev. Lett. **95**, 197401 (2005)

[3] C. D. Spataru *et al.*, Phys. Rev. Lett. **95**, 247402 (2005)