HL 17: Focussed Session: Atomic Scale Characterization

For a detailed understanding of complex semiconductor nano- and heterostructures as well as the physics of devices based on them, a systematic determination and correlation of the structural, chemical, electronic, and optical properties on a nanometer or atomic scale is essential. This session brings the atomic structural and chemical imaging using scanning tunneling microscopy, atomic probe tomography, and ultra-high resolution transmission electron microscopy together with the nanoscopic mapping of the optical and electronic properties using scanning transmission microscopy cathodoluminescence spectral imaging.

Organizers: Holger Eisele(TU Berlin), Frank Bertram and Jürgen Christen (OvGU Magdeburg)

Time: Tuesday 9:30–13:00 Location: EW 202

Invited Talk HL 17.1 Tue 9:30 EW 202

Quantitative Electron Microscopy for III/V on Silicon integration — •Kerstin Volz — Philipps-Universität Marburg, Department of Physics and Materials Science Center, Marburg, Germany

Integration of active III/V devices on Silicon substrates tremendously increases the functionality of this semiconductor material. In order to realize true monolithic integration, a defect-free nucleation layer is of outmost importance. Moreover, the exact atomic structure of the interface as well as of possible defects, like antiphase domains, is important as they have a decisive impact on charge carrier characteristics and band alignment at the interface. In this presentation several electron microscopic techniques will be explained, which are used to derive not only the quantitative atomic arrangement across a heterointerface, but also the local as well long-range electric field at and across interfaces. These techniques include high angle annular dark field STEM (Scanning Transmission Electron Microscopy), which allows - after appropriate simulation of the scattering process - to gain the three-dimensional quantitative composition. Complementary to this, in 4D STEM a fast pixelated detector is used to obtain information on electric fields. Both techniques, which are operated in an aberration-corrected microscope, will be applied to GaP/Si specimens, grown by metal organic vapour phase epitaxy under highly different conditions, to derive information on the exact structure of interfaces and defects.

Invited Talk HL 17.2 Tue 10:00 EW 202

Total Tomography of Nonplanar Heterostructures: Doping and Confinement Pontentials — •Lincoln Lauhon — Northwestern University, USA

The direct visualization of nanoscale structure enables the development of predictive models of novel physical behaviors. The talk will discuss recent advances in the nanoscale tomography of non-planar III-As semiconductor heterostructures including narrow gap III-As nanowire and related heterostructures for next generation compact light sources and novel computing schemes. Atom probe tomography is used to visualize the distribution of atoms in three dimensions with nanoscale resolution, providing new insights into growth mechanisms and the resulting the distribution of dopant atoms. Of particular interest is the evolution of composition of AlGaAs barrier layers and InGaAs quantum wells and nanowires when multiple growth facets are present. Generically, we find that alloy composition and doping rates vary considerably with surface faceting and polarity. Three-dimensional maps of the composition, when combined with appropriate models, reveals how the confinement of electrons and photons is influenced by size, shape, and interfaces, providing a foundation for device engineering. The tomography effort has recently been expanded to include 3-D mapping of strain using x-ray Bragg projection ptychography. The novel combination of atom probe tomography and x-ray ptychography illuminates a route to the total tomography of nanostructures.

HL 17.3 Tue 10:30 EW 202

Atomic Scale Investigation of Near Interface Defects at the SiC/SiO$_2$-Interface: Microscopy, Atom Probe Tomography and Theory — •Dipanwita Dutta[1,2], Deb De[2], Elisabeth Müller[1], Stephan Gerstl[3], Stefan Goedecker[2], Holger Bartolf[5], Jörg Lehmann[5], Giovanni Alfieri[5], Massimo Camarda[1], Adolf Schöner[4], and Thomas Jung[1,2] — [1]Paul Scherrer Institute, Switzerland — [2]University of Basel, Switzerland — [3]ETH Zürich, Switzerland — [4]Ascatron, Kista, Sweden — [5]ABB Switzerland Ltd, Corporate Research Baden Dättwil, Switzerland

SiC is in many aspects superior to Si. SiC MOSFETs, however, are compromised by low channel mobilities due to the poor quality of the SiC/SiO$_2$ interface after thermal oxidation, the method of choice for fabrication. Defects occur near the SiC/SiO$_2$ interface due to the complex thermal oxidation process for SiC in comparison to Si which requires removal of carbon in the form of CO and CO_2. We identify the most relevant defects for degrading the MOS performance. We analyzed near-oxide defects at different stages of fabrication and passivation by DFT-based theory and by experimental means. Atomic Force Microscopy (AFM), performed after oxide removal, reveals smoother interfaces near N_2O passivated oxides as compared to the O_2 processed oxides. Raman spectroscopy of the buried interface shows clear evidence for unwanted carbon for the first time. Electron Microscopy and Local Electrode Atom Probe (LEAP) data, will be shown at the conference along with theoretical approaches to explain the carbon-cluster formation.

HL 17.4 Tue 10:45 EW 202

A three dimensional structural model of antiphase domains in GaP on Si(001) — •Pascal Farin[1], Malte Marquardt[1], Celina S. Schulze[1], Wjatscheslav Martyanov[1], Andreas Beyer[1], Kerstin Volz[2], and Andrea Lenz[1] — [1]Technische Universität Berlin, Institute of Solid State Physics, 10623 Berlin, Germany — [2]Philipps-Universität Marburg, Materials Science Center, 35032 Marburg, Germany

The integration of III/V-semiconductors on Si(001) has been a long standing research aim to lower the cost of optoelectronic devices and simultaneously improve their performance. Because there is only a small lattice mismatch between Si and GaP, this particular III/V semiconductor is used preferentially. However, due to charged defects called antiphase domains (APDs) in GaP forming at the interface, this has proven to be quite challenging. While the search for growth conditions to avoid their formation has been successful, their exact shape remains unclear. In this work APDs in GaP on Si(001) are investigated by means of cross-sectional scanning tunneling microscopy (XSTM). This method offers unique insight into the appearance of APDs due to its high surface sensitivity. Two perpendicular cross sections of a GaP/Si sample are investigated to develop a three dimensional model for the APDs.

This work is supported by the DFG, project LE 3317/1-2.

HL 17.5 Tue 11:00 EW 202

Structural and electronic properties of AlkInSe2/CuInSe2 (Alk = K, Rb, Cs) interfaces from density functional theory calculations — •Maria Malitckaya, Hannu-Pekka Komsa, Ville Havu, and Martti Puska — Department of Applied Physics, Aalto University, P.O. Box 11000, Espoo, Finland

The efficiency of Cu(In, Ga)Se$_2$ (CIGS) - based solar cells has increased very fast, thanks to the alkali post deposition treatment (PDT). The latest record efficiency of CIGS solar cells has been achieved by using heavy alkali (K, Rb, and Cs) PDT. After K, Rb, and Cs PDT, chalcopyrite solar cells exhibit improved junction quality, open-circuit voltages and fill factors. However, the physical reasons behind these effects are still under discussion. At the microscopic level CIGS absorbers demonstrate changes in surface composition and morphology after Alk PDT. This effect has been associated with formation of Alk-In-Se secondary phases. Using first-principles calculations within the density functional theory, we have considered the role of alkali metal atoms in the efficiency enhancement. We have investigated the most important parameters of AlkInSe$_2$ phases, secondary phase formation during the PDT process and AlkInSe$_2$/CuInSe$_2$ interfaces.We have found that conduction band offsets are small for all orientations of the

interfaces. The increase of the surface band gap seen in XPS measurements can be explained by the formation of $AlkInSe_2$ phases. In the case of K-PDT the measured band gap of 2.5 eV is consistent with the calculated value for monoclinic $KInSe_2$.

15 min. break.

Invited Talk HL 17.6 Tue 11:30 EW 202

Modulating electron beams in space and time to probe for genuine structures and function at the atomic scale — •Christian Kisielowski — Lawrence Berkeley National Laboratory

n high resolution electron microscopy objects are actively altered by the intense electron irradiation that is necessary to reach single atom sensitivity. In these circumstances a control of beam-sample interactions is no longer a commodity but a necessity. Therefore, it is of outstanding interest to develop new tools and concepts that strive for a stricter control of the probing electron beam in space and time in order to optimize the detection of every scattering event.

This contribution describes research that aims at exploiting the emerging ability to better understand layered semiconductors and other nano-materials containing soft and hard matter components by directly determining their atom arrangement in three-dimensions using low-dose rate electron microscopy. The approach mimics best practices in biological research by capturing series of entirely noise dominated images with dose rates that can be smaller than 20 e/Å2s, which are successively reconstructed to obtain in-line holograms with unprecedented contrast and resolution.

In such images we observe a variety of previously unknown atom configurations that are otherwise hidden behind a barrier of beam-induced object alterations and capture radiation sensitive structures at atomic resolution even if they are greatly affected by an exposure of the material to water vapor or other gases. Recent progress with time resolved electron microscopy further accelerates the progress.

Invited Talk HL 17.7 Tue 12:00 EW 202

Advanced Nano-scale Characterization of Nitrides using Helium Temperature Scanning Transmission Electron Microscopy Cathodoluminescence — •Gordon Schmidt — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

For a detailed understanding of complex semiconductor heterostructures and the physics of devices based on them, a systematic determination and correlation of the structural, chemical, electronic, and optical properties on a nanometer scale is essential. Luminescence techniques belong to the most sensitive, non-destructive methods of semiconductor research. The combination of luminescence spectroscopy * in particular at liquid He temperatures - with the high spatial resolution of a scanning transmission electron microscopy (STEM) ($<$ 1 nm at RT, $<$ 5 nm at 10 K), as realized by the technique of low temperature scanning transmission electron microscopy cathodoluminescence microscopy (STEM-CL), provides a unique, extremely powerful tool for the optical nano-characterization of semiconductors, their heterostructures as well as their interfaces. Typical results which will be presented include nm-scale correlation of the optical and structural properties as well as appearance of structural defects in nitride based nanostructures.

Invited Talk HL 17.8 Tue 12:30 EW 202

Tip-enhanced Raman spectroscopy in semiconductor nanostructures and graphene — Emanuele Poliani[1] and •Janina Maultzsch[1,2] — [1]Technische Universität Berlin, Germany — [2]Friedrich-Alexander-Universität Erlangen

Tip-enhanced Raman spectroscopy provides spatial resolution beyond the diffraction limit and is therefore useful for application in the characterization of semiconductor nanostructures. We will present experimental results on group-III nitride nanostructures and on graphene-based materials. In a doped GaN DBR structure, we investigate the carrier dependence of the Raman signal and the periodicity of the structure. In isotopically modified graphene with 12C and 13C regions, we discuss our investigations of the interface between the two regions and of superlattice structures. Finally, we show in carbon nanotubes that the strong polarization dependence present in conventional Raman scattering is almost absent in TERS.