

## MM 9: Topical Session TEM III

Time: Monday 15:45–17:30

Location: IFW A

**Topical Talk**

MM 9.1 Mon 15:45 IFW A

**Advanced electron microscopy and first-principles calculations: New insights into materials science on the atomic scale** — ●ROLF ERNI — Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

New electron optical devices, such as monochromators, spherical and chromatic aberration correctors, have boosted the resolution in (scanning) transmission electron microscopy. In parallel, the revolutionized optics has increased the sensitivity of the imaging techniques to a level where, for instance, the dynamics of individual atoms can be monitored, employing a microscope setting tailored to the material to minimize radiation damage. This overall progress has opened the possibility to reliably study smaller materials systems; while typically in conventional microscopy millions of atoms constitute a high-resolution micrograph, the new optics allows for monitoring systems that are merely defined by a few hundred atoms, which indeed is a requirement if the functionality of a nano-device needs to be analyzed. As a consequence, nowadays microscopy data can provide direct input for first-principles calculations. Indeed, combining the theoretical and the experimental approach leads to synergies that simplify finding answers for new observations. The advantage of this tandem approach is demonstrated by discussing the dynamics and stability of ad-atoms and ad-molecules on suspended graphene. Moreover, while most atomic-scale studies are confined to two-dimensional projections, an outlook is given on how the third spatial dimension could be explored.

**Topical Talk**

MM 9.2 Mon 16:15 IFW A

**Quantitative STEM: Composition mapping in InGaN** — ●ANDREAS ROSENAUER<sup>1</sup>, THORSTEN MEHRTENS<sup>1</sup>, KNUT MÜLLER<sup>1</sup>, KATHARINA GRIES<sup>1</sup>, MARCO SCHOWALTER<sup>1</sup>, STEPHANIE BLEY<sup>1</sup>, PARLAPALLI VENKATA SATYAM<sup>1</sup>, CHRISTIAN TESSAREK<sup>1</sup>, KATHRIN SEBALD<sup>1</sup>, MORITZ SEYFRIED<sup>1</sup>, JÜRGEN GUTOWSKI<sup>1</sup>, ADRIAN AVAMESCU<sup>2</sup>, KARL ENGL<sup>2</sup>, and STEPHAN LUTGEN<sup>2</sup> — <sup>1</sup>Universität Bremen, Institut für Festkörperphysik, D-28359 Bremen — <sup>2</sup>OSRAM Opto Semiconductors GmbH, D-93055 Regensburg

In this contribution we demonstrate that measurement of In concentration in InGaN layers is possible by scanning transmission electron microscopy Z-contrast imaging as the tendency to form In rich regions due to electron beam irradiation is smaller than for parallel beam illumination. The suggested method is based on comparison of intensity normalized with respect to the incident electron beam with image simulation computed with the STEMsim program. In InGaN, static atomic displacements are caused by the different covalent radii of the metal atoms. These displacements are computed by structure optimization of InGaN supercells using empirical potentials in the Stillinger Weber parameterization. The suggested procedure is validated using an InGaN layer with 7 % homogeneous In concentration by comparison of the STEM results with results obtained by other methods. Despite a high convergence angle of the incident electron beam, simulation of an abrupt interface between InGaN and GaN shows that artificial blurring of the interface is significantly reduced by electron channelling.

MM 9.3 Mon 16:45 IFW A

**TEM studies of PbS-ZnS/ZnO quantum confinement structures for solar cells** — ●PETER G. SCHINDLER<sup>1</sup>, NEIL P. DASGUPTA<sup>2</sup>, ORLANDO TREJO<sup>2</sup>, CHRISTIAN RENTENBERGER<sup>1</sup>, THOMAS WAITZ<sup>1</sup>, FRITZ B. PRINZ<sup>2</sup>, and HANS-PETER KARNTHALER<sup>1</sup> — <sup>1</sup>University of Vienna, Physics of Nanostructured Materials, Boltzmannngasse 5, 1090 Wien, Austria — <sup>2</sup>Stanford University, Dept. of Mechanical Engineering, Stanford, CA 94305, USA

Research to maximize the efficiency of solar cells used for photovoltaic power generation is a timely issue. Si technology uses only a limited range of frequencies of the solar spectrum. To overcome this, quantum confinement solar cells give the opportunity for band gap engineering

by quantum effects facilitated by dimensions in the nm range. We report on a transmission electron microscopy (TEM) study of layers of PbS and ZnS/ZnO deposited by atomic layer deposition. To prepare cross-section TEM samples the structures were glued together face to face to protect them. To achieve wedge shaped TEM foils with an extremely shallow angle the samples were mechanically polished and in a last step softly polished with Ar<sup>+</sup> ions. The cross-sectioned multilayer quantum dot (QD) structure, its composition and morphology were investigated with different TEM techniques, e.g. high resolution TEM, and high angle annular dark field. The results are: The size of the QDs is in the range of the thickness of the layers which is about 2-5 nm. The QDs are faceted and either of small round shape or elongated along the layers. The range of size variations of the QDs increases with distance from the substrate resulting in the desired variation of band gaps.

MM 9.4 Mon 17:00 IFW A

**Annealing in InGaNs studied by TEM three-beam imaging** — ●KNUT MÜLLER<sup>1</sup>, MARCO SCHOWALTER<sup>1</sup>, MICHAEL HETTERICH<sup>2</sup>, DONGZHI HU<sup>2</sup>, DANIEL SCHAADT<sup>2</sup>, PHILIPPE GILET<sup>3</sup>, KERSTIN VOLZ<sup>4</sup>, and ANDREAS ROSENAUER<sup>1</sup> — <sup>1</sup>Univ. Bremen, D-28359 Bremen — <sup>2</sup>Karlsruhe Inst. of Techn., D-76131 Karlsruhe — <sup>3</sup>CEA-LETI, F-38054 Grenoble — <sup>4</sup>Univ. Marburg, D-35032 Marburg

A 3-beam TEM image formed by 000, 200, and 220 is used for simultaneous atomic-scale measurement of In and N in an In<sub>0.28</sub>Ga<sub>0.72</sub>N<sub>0.02</sub>As<sub>0.98</sub> quantum well. In this setup, subsequent diffractogram filtering yields 200 and 220 lattice fringes that are not coupled by nonlinear imaging. Images are acquired with a FIB-fabricated, L-shaped objective aperture in a Cs-corrected Titan 80/300. Indium and nitrogen contents are determined by comparing chemically sensitive 200 fringe amplitude and 220 strain with simulated reference data., which includes bonding and static atomic displacements (SAD). It is demonstrated that bonding improves accuracy up to 30%, and that SAD cause absorption in Bragg beams due to Huang scattering, which is treated by additional absorptive form factors. For the present structure, annealing is shown to cause photoluminescence to increase by a factor of 20 and to blue-shift by 65nm. Using our 3-beam method, this can be assigned to a dissolution of In- and N-rich regions in favour of a homogenisation of layer thickness and -stoichiometry.

MM 9.5 Mon 17:15 IFW A

**Quantitative evaluation of Avrami-type crystallization in a thin GeSi film using double wedge geometry** — ●FLORIAN NIEKIEL and ERDMANN SPIECKER — CENEM, Universität Erlangen-Nürnberg, Erlangen, Germany

A key to understanding and controlling thin film growth processes and properties is the knowledge of the variation in structure with distance from the substrate. Transmission electron microscopy (TEM) is known as a powerful tool for characterization of thin films structures. By combining plan-view and cross-section analysis a qualitative view of the three-dimensional (3D) film structure can be obtained. However, neither of the two geometries is compatible with the need for quantitative characterization of the structural, crystallographic or compositional parameters that define the thin film. We have recently developed a new double wedge sample preparation technique that enables plan-view TEM investigation of large areas at each depth in the film. Based on a quantitative evaluation of image series statistically relevant data on the 3D film structure can be obtained. Here, we demonstrate the technique for a GeSi film that first started to grow in the amorphous state, then formed crystalline nuclei that expanded with increasing distance from the substrate finally replacing all amorphous material in the top part of the film. Quantitative evaluation of extensive image series obtained in double wedge geometry allowed us to determine the relative fraction of crystalline material as a function of distance from the substrate.