

O 19: Semiconductor Substrates: Structure, Adsorption and Growth

Time: Monday 17:00–19:30

Location: Poster A

O 19.1 Mon 17:00 Poster A

Epitaxial Growth of Ultrathin Lead Films on Silicon (111) — •TOBIAS WITTE, TIM FRIGGE, BERND HAFKE, BORIS KRENZER, and MICHAEL HORN-VON HOEGEN — Department of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Epitaxial growth of ultrathin Pb films on Si(111) was studied by means of high resolution electron diffraction (SPA-LEED). The $\beta(\sqrt{3}\times\sqrt{3})$ reconstruction with 1/3 ML Pb-coverage (1 ML $\hat{=}$ 1 Pb atom per Si surface atom = 7.84×10^{14} Pb atoms/cm²) was prepared by desorption of a larger amount of Pb at 450 °C and used as a template layer for deposition. The layer-by-layer growth mode of Pb for coverages larger than 3 ML was confirmed through LEED intensity oscillations during deposition at low temperatures of 100 K. In the coverage regime of 1-3 ML the diffracted intensity is strongly reduced, indicating roughening of the strained Pb film. Films with 3-5 ML thickness are laterally relaxed through a network of interfacial misfit dislocations which is observed through satellite spots surrounding all integer order spots in the diffraction pattern. A $G(S)$ -analysis indicates an increased vertical layer distance of 3.05 Å, which relaxes towards the bulk-like value of 2.87 Å for films of 6 or more ML thickness. This behavior is corroborated through the LEED intensity oscillations during deposition, which were measured at different diffraction conditions (i.e. different electron energies). Films deposited on the $\beta(\sqrt{3}\times\sqrt{3})$ reconstruction exhibit a slight azimuthal disorder, which is reflected through banana-like distorted integer order spots in the diffraction pattern. These films are metastable and form islands at temperatures above 220 K.

O 19.2 Mon 17:00 Poster A

Growth, structure and morphology of NiGe and SnGe nanostructures on Ge(001) — •NICOLAS BRAUD¹, SIMON FISCHER¹, INGA HEIDMANN¹, THOMAS SCHMIDT¹, JAN INGO FLEGE¹, TOMASZ GRZELA², THOMAS SCHROEDER², and JENS FALTA¹ — ¹Institute of Solid State Physics, University of Bremen, Germany — ²Leibniz Institute of Innovative Microelectronics (IHP), Frankfurt (Oder), Germany

Nickel germanide is a promising candidate as a contact material in MOSFETs and is expected to play an important role in future Ge-based electronics due to its low formation temperature and low resistivity. In this context, SnGe can be used as channel material to improve the CMOS performance, as it has an even higher carrier mobility than Ge. Here we present an in-situ investigation of the growth of nickel germanide and SnGe at various temperatures on the Ge(001) surface by means of low-energy electron microscopy (LEEM) and micro diffraction (μ LEED). We observe the growth of compact and elongated islands along two orthogonal directions after nickel deposition at 450 °C and 530 °C. We also show that with increasing temperature, the size of the NiGe islands increases while the island density drastically decreases, showing an Arrhenius like behavior [1]. Subsequent thermal annealing above 600 °C results in the dissolution of the NiGe islands into the bulk substrate. Finally we compare the results obtained with the NiGe and those obtained with SnGe.

[1] T. Grzela et al., *Nanotechnology* **26**, 385701 (2015)

O 19.3 Mon 17:00 Poster A

Hydrogen etching of SiC(0001): STM study of an epitaxy template — •MAXIMILIAN BAUERNFEIND, FELIX REIS, STEFAN GLASS, JULIAN AULBACH, RALPH CLAESSEN, and JÖRG SCHÄFER — Physikalisches Institut und Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

The hexagonal (0001) surface of silicon carbide (SiC) offers a huge playground for the epitaxy of a large variety of different materials, which has received little attention until now. One challenging aspect is the growth of high- Z atom lattices made out of, e.g., Sn or Bi in the monolayer regime, which may potentially form graphene analogs with a hexagonal structure. Because of the strong spin-orbit coupling in this class of materials, topological protected edge states can emerge. To enable epitaxy of such promising high- Z materials, one has to focus on the substrate quality, and prepare defect-free and well-ordered flat surfaces. In-situ gas phase etching can thereby attack the inert SiC much better than chemical pathways. It is performed at temperatures above 1000 °C in a hydrogen atmosphere.

To get new insights of this substrate on the atomic scale, we will ad-

dress in general the differences between the etching treatments in a stationary and a flowing hydrogen atmosphere by means of scanning tunneling microscopy. To be specific, we will demonstrate the effects of different hydrogen flow values, including addition of the inert gas helium, as well as the influence of the substrate temperature. The results will be analyzed regarding large-scale terrace formation and defect density.

O 19.4 Mon 17:00 Poster A

Growing mechanism and tip-induced switching of acetylbiphenyl on Si(100)-(2x1):H — •FRANK EISENHUT¹, JUSTUS KRÜGER¹, ANJA NICKEL¹, XAVIER BOUJU³, GIANAURELIO CUNIBERTI^{1,2}, and FRANCESCA MORESCO¹ — ¹Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, — ²Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany — ³CNRS, CEMES (Centre d'Elaboration des Matériaux et d'Etudes Structurales), Toulouse, France

The investigation of molecules on semiconducting surfaces has caused much effort and can push forward molecular electronic devices. In this context one approach is to exploit the structure and related properties of the molecules and to use them as electronic components. In this study one candidate for a molecular latch, acetylbiphenyl (ABP), was investigated by means of low-temperature scanning tunneling microscopy on the passivated silicon surface. Firstly here we report on the growing mechanisms of ABP on Si(100)-(2x1):H. The molecule is fulfilling a dangling bond initiated growing mechanism along as well as perpendicular to the silicon dimer rows and consequently it is forming a 1-dimensional molecular assembly. Despite the growing of the molecule we found a reversible tip-induced conformational change of a molecule at the end of the grown molecular chain. This molecular change can be possibly used as a switch on this surface.

O 19.5 Mon 17:00 Poster A

Real-space investigation of the reaction channels of acetylene on Si(001) — PATRICK KIRSTEN, •CHRISTIAN LÄNGER, and MICHAEL DÜRR — Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, 35392 Giessen

Ethylene and acetylene adsorption on Si(001) are benchmark systems for the understanding of adsorbate reactions on semiconductor surfaces. In the case of ethylene, the [2+2] cycloaddition proceeds via a mobile precursor state; in the final state the ethylene molecule is adsorbed either on top of one dimer or bridging two neighbored dimers of one dimer row. Due to different conversion barriers from the precursor into the final state, the on-top configuration is favored by a factor of ten at room temperature [1]. Early experiments on acetylene adsorption also report a precursor-mediated reaction channel [2]. On the other hand, DFT calculations suggest the existence of a direct reaction pathway for C₂H₂ on Si(001) [3].

In order to resolve this contradiction, we performed STM measurements after adsorption of acetylene at different surface temperatures. The ratio of on-top to end-bridge configurations is found to depend on surface temperature. From the temperature dependence, a precursor-mediated reaction is concluded and the barrier difference for the two reaction channels is calculated.

[1] Mette, et al., *Chem. Phys. Lett.* **483**, 209 (2009).

[2] Clemen, et al., *Surf. Sci.* **268**, 205 (1992).

[3] Cho and Kleinmann, *Phys. Rev. B* **69**, 075303 (2004).

O 19.6 Mon 17:00 Poster A

High Resolution Electron Energy Loss Spectroscopy of Ammonia Adsorbed on a Water Reacted Si(001)-(2x1)-Surface — NIKLAS FORNEFELD¹, •FELICITAS SCHOLZ¹, FRANCOIS ROCHET³, STEFAN KUBSKY², and ULRICH KÖHLER¹ — ¹AG Oberflächenphysik, Ruhr-Universität Bochum, Germany — ²Synchrotron Soleil, St. Aubin (Paris), France — ³Laboratoire de Chimie Physique Matière et Rayonnement, Univ. P. et M. Curie, Paris, France

Surface bound hydroxyl-groups on silicon surfaces became an interesting topic for research due to their use as interface between an anorganic and an organic semiconductor. To investigate the binding properties (e.g. pKa-value) on those silanol-groups we studied the adsorption of ammonia (NH₃) as an example for a Lewis base. In order to verify the

adsorption geometry and the behavior during the process of unfreezing, that had been proposed on the basis of XPS/NEXAFS studies, we studied the $\text{NH}_3/(\text{H}/\text{OH})/\text{Si}(001)-(2\times 1)$ system with HREELS at 125 K and 300 K. We report the self-limited adsorption of molecular ammonia on surface silanols in a proton-acceptor geometry (NH_3 giving lone pair to Si-OH) at 125 K. The saturation coverage was found to be smaller than one monolayer. In addition there were indications for the growth of a small amount of SiNH_2 (dissociation of NH_3) that seems to increase with higher dosage up to 17 L. At 300K (after unfreezing) the molecularly bound ammonia completely desorbs due to weak bonding while the behavior of SiNH_2 could not finally be cleared up.

O 19.7 Mon 17:00 Poster A

Sub-surface Incorporation of 3d Metal Atoms Into Bi(111) Films — •N.J. VOLLMERS¹, C. KLEIN², G. JNAWALI², D. LÜKERMANN³, C. TEGENKAMP³, H. PFNÜR³, M. HORN-VON HOEGEN², W.G. SCHMIDT¹, and U. GERSTMANN¹ — ¹Theoretische Physik, Universität Paderborn — ²Fakultät für Physik, Universität Duisburg-Essen — ³Institut für Festkörperphysik, Leibniz Universität Hannover

Substrate-stabilized Bi(111) bilayers and Bi(111) surfaces have been studied intensively due to the occurrence of strongly spin-orbit split surface states. The Bi(111) surface provides a well-defined incorporation site in the first bilayer that traps highly coordinating atoms like transition metals (TMs) or noble metals [1].

Here we use density functional theory (DFT) to gain a microscopic insight into the sub-surface incorporation and its implication for the Bi surface electronic properties. The Quantum-ESPRESSO package is used for relativistic DFT calculations. Thereby, spin-orbit coupling effects are included by using a numerically efficient PAW-based implementation [2]. It is found that 3d TMs penetrate the surface barrier-free, thereby causing no morphological changes at the surface. Isolated atoms assume a seven-fold coordinated interstitial position, and provide metallic near-surface state. Furthermore, we investigate the interaction between these subsorbates by analyzing subsorbate densities up to one impurity per Bi(111) unit cell. Interestingly in comparison to the single impurity, the Bi(111) lattice is restored to its ideal form.

[1] C. Klein et al., Phys. Rev. B 91, 195441 (2015).

[2] U. Gerstmann et al., Phys. Rev. B 89, 165431 (2014).