O 38 Halbleiteroberflächen und -grenzflächen

Zeit: Dienstag 10:45–13:00 Raum: TU EB301

O 38.1 Di 10:45 TU EB301

Atomic structure of the GaAs(001)-$c(4 \times 4)$ surface: first-principles evidence for diversity of heterodimer motifs — •E. Penev[1,2], P. Kratzer[1], and M. Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, D-14195 Berlin — [2]Institut für Physik, Universität Basel, CH-4056 Basel, Schweiz

The atomic structure of the $c(4 \times 4)$ reconstruction, formed on the GaAs(001) surface under high arsenic overpressure, has recently been attracting renewed interest. This has lead to a revision of the commonly accepted $c(4 \times 4)$ structural model but a definitive understanding of the driving force for the newly proposed structure[1] was lacking. Targeting the later problem, the talk will present a state-of-the-art theoretical study of the GaAs(001)-$c(4\times4)$ surface employing *ab initio* atomistic thermodynamics based on density-functional theory calculations. We shall demonstrate[2] that in a range of stoichiometries, between those of the conventional three As-dimer and the new three Ga-As dimer model[1], there exists a diversity of atomic structures featuring Ga-As heterodimers, *driven by surface configurational entropy*. These results fully explain the experimental scanning tunneling microscopy images and are likely to be relevant also to the $c(4 \times 4)$-reconstructed (001) surfaces of other III-V semiconductors.

[1] A. Ohtake *et al.*, Phys. Rev. Lett. **89**, 206102 (2002).
[2] E. Penev *et al.*, Phys. Rev. Lett. **93**, 146102 (2004).

O 38.2 Di 11:00 TU EB301

InP growth on $c(4 \times 4)$ and (1×3) reconstructed GaAsSb(100) surfaces — •Z. Kollonitsch[1], U. Seidel[1], S. Neumann[2], F.-J. Tegude[2], F. Willig[1], and T. Hannappel[1] — [1]Hahn-Meitner-Institut, SE 4, Glienicker Strasse 100, D-14109 Berlin — [2]Universität Duisburg/Essen, Halbleitertechnik/Halbleitertechnologie, Lotharstr. 55, ZHO, Gebäude LT, D-47048 Duisburg

Lattice matched $GaAs_{0.5}Sb_{0.5}$/InP(100)-layers were grown by MOVPE at 770K. Contamination free sample transfer into ultrahigh vacuum (UHV) allowed for the correlation of in-situ reflectance anisotropy/difference (RA/RD) spectra with LEED and photoelectron spectra (XPS/UPS). The in-situ signals indicated that the $GaAs_{0.5}Sb_{0.5}$ surface was Sb-rich during growth and turned preferably into an As-rich surface after growth. The group-V rich surface reconstructions formed $c(4 \times 4)$ and (1×3) symmetries, which are well known from the related binaries GaAs and GaSb. Energy dependent UP spectra of the $c(4 \times 4)$ reconstruction showed a prominent peak near the valence band maximum which was attributed to a surface state. There were similarities between the $c(4 \times 4)$ reconstructed surfaces of $GaAs_{0.5}Sb_{0.5}$ and GaAs. XPS measurements of InP/GaAsSb interfaces taken in UHV and I-V curves of InP/GaAsSb resonant tunneling diodes indicated that Sb segregation into a subsequent InP layer was significantly lower when the InP film was grown on the $c(4 \times 4)$ reconstructed $GaAs_{0.5}Sb_{0.5}$ surface compared to the (1×3) reconstructed surface.

O 38.3 Di 11:15 TU EB301

A study on the surface structure of CuInSe2 (001) — •Thalia Deniozou[1], Norbert Esser[1], Thomas Schulmeyer[2], and Ralf Hunger[2] — [1]Institute for Analytical Sciences, Albert-Einstein-Str. 9, 12489 Berlin-Adlershof, Germany — [2]Surface Science Division, Institute of Materials Science, Darmstadt University of Technology, Petersenstr. 23, 64287 Darmstadt, Germany

In contrast to most other semiconductor surfaces the atomic structure of chalcopyrite (001) surfaces is practically unresolved. Reconstructions have not been reported yet. The (001) surface structure of the chalcopyrite semiconductor CuInSe2 was studied by means of Low Energy Electron Diffraction, Auger Electron Spectroscopy and Synchrotron X-ray Photoelectron Spectroscopy. For the study heteroepitaxial CuInSe2/GaAs (001) films were employed which were grown by molecular beam epitaxy and capped with a protective Se layer. The CuInSe2 surfaces were initially decapped and then treated by simultaneous Ar+-ion bombardment and annealing. Two different reconstructions in dependence of the preparation time were observed for the first time, namely a (2x4) and a mixed (2x4)/(4x2) reconstruction. The chemical state and composition of the CuInSe2(001) surfaces were monitored by the photoelectron spectra of the Cu2p, Se3d, and In4d core levels. The observed surface core level shifts are discussed in relation to possible surface geometries.

O 38.4 Di 11:30 TU EB301

Electronic structure of Ge(001) surface studied by room temperature scanning tunneling spectroscopy — •Oguzhan Gurlu[1,2], Harold J.W. Zandvliet[1], and Bene Poelsema[1] — [1]Solid State Physics Group, MESA+ Research Institute, University of Twente, PO. Box. 217, 7500AE Enschede, The Netherlands — [2]Max-Planck Institut fur Festkorperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

The surface electronic structure of Ge(001) has been studied by scanning tunneling spectroscopy. The measured surface densities of states unequivocally reveals the presence of a metallic state on the (2x1) domains, which is absent on the c(4x2) domains. This metallic state, so far only observed in integral measurements, is attributed to the flip-flopping dimers, which constitute the (2x1) domains. Our data also reveals a set of previously unresolved surface states, in perfect agreement with published theoretical predictions.

O 38.5 Di 11:45 TU EB301

Photoelektronenbeugungsuntersuchungen an der SiO_2/4H-SiC(0001)-Grenzfläche — •Mark Schürmann, Stefan Dreiner, Ulf Berges, Daniel Weier, Abner de Siervo und Carsten Westphal — Universität Dortmund, Experimentelle Physik 1, Otto-Hahn-Straße 4, 44221 Dortmund

Thermisch oxidierte Siliziumkarbidoberflächen wurden mittels Photoelektronenbeugung untersucht. Dazu stand intensives Synchrotronlicht mit hoher Energieauflösung zur Verfügung, so daß es möglich war, die lokale atomare Struktur der verschiedenen chemisch verschobenen Komponenten im Si2p-Photoemissionsspektrum getrennt zu untersuchen. Insbesondere war so das Signal der Siliziumatome an der Siliziumoxid/Siliziumkarbid-Grenzfläche der Analyse zugänglich.

Die Ergebnisse der Messungen zeigen, daß auch thermisch oxidierte Proben, die keine langreichweitige Ordnung zeigen, an der Grenzfläche lokal durchaus geordnet sein können. Ein Vergleich mit Messdaten von einer Probe mit geordneter Silikatschicht zeigt, daß die lokale atomare Struktur in der Umgebung der Grenzflächenatome in beiden Proben gleich ist.

O 38.6 Di 12:00 TU EB301

Diffusion Pathways of Hydrogen across the Steps of a vicinal Si(001)-Surface — •P. Kratzer[1], M. Lawrenz[2], C. Schwalb[2], M. Dürr[2], and U. Höfer[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, D-14195 Berlin — [2]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

Surface diffusion of hydrogen on vicinal Si(001) surfaces is an interesting system to test theoretical results against experimental data, because selective hydrogen adsorption *at the step sites only* opens the experimental possibility to prepare a well-defined initial state. Diffusion of H away from the D_B step sites has been observed by real-space STM studies at elevated temperatures. We have investigated the diffusion pathways by performing density-functional theory calculations using the gradient-corrected PW91 functional and the plane-wave+pseudopotential approach. While H atoms bind more strongly to the lower terrace sites than to the upper terrace sites, the calculated energy barriers show that H diffusion onto the upper terrace is strongly preferred, in agreement with the experimental findings. We learn from the calculations that a metastable intermediate where hydrogen binds weakly to an already fourfold coordinated Si atom at the step is responsible for the lowering of the "upward"diffusion barrier.

O 38.7 Di 12:15 TU EB301

Untersuchung der Struktur der SiO_2/Si-Grenzschicht in Abhängigkeit von der Oberflächenorientierung — •Stefan Dreiner, Mark Schürmann, Ulf Berges, Martin Krause, Christian Flüchter und Carsten Westphal — Universität Dortmund, Experimentelle Physik I, 44221 Dortmund

Die Methode der Photoelektronenbeugung benötigt im Gegensatz zu vielen anderen Beugungsmethoden keine perfekte Periodizität, um Informationen über die lokale atomare Struktur zu gewinnen. Daher ist

sie ideal zur Untersuchung des Übergangs zwischen kristallinem Silizium und seinem amorphen Oxid.
Die untersuchten Grenzschichten wurden auf Si-Proben mit (100)-,(111)- und (110)-Orientierung durch thermische Oxidation hergestellt (wenige Å SiO_2-Schichtdicke). Am U41-PGM Meßplatz bei BESSY II wurden hochaufgelöste Si2p-Photoemissionsspektren über nahezu den gesamten Halbraum bei einer Photonenenergie von $h\nu = 180$ eV aufgenommen. Diese Spektren ermöglichen die Trennung der verschieden Oxidationsstufen des Siliziums (Si^{1+}, Si^{2+}, Si^{3+}, Si^{4+}) vom Volumensignal (Si^{B}). Aus den Intensitäten der Si^{x+}-Signale in Abhängigkeit vom Polarwinkel ergibt sich die Tiefenverteilung der Oxidationsstufen in der Grenzschicht. Die Si^{x+}-Beugungsmuster liefern weitere Informationen über die atomare Umgebungsstruktur der Si-Oxidationsstufen. Die Daten der verschiedenen Oberflächenorientierungen werden miteinander verglichen.

O 38.8 Di 12:30 TU EB301

Investigation of the geometrical properties of NiMnSb-Half-Heusler thin films. — •Andreas Stahl[1], Christian Kumpf[1], Eberhard Umbach[1], Peter Bach[2], Georg Schmidt[2], and Laurens Molenkamp[2] — [1]Experimentelle Physik II, Univ. Würzburg — [2]Experimentelle Physik III, Univ. Würzburg

The Half-Heusler alloy NiMnSb is an interesting material which may be used in spintronic devices due to its unusual half-metallic properties. It can be grown in high crystalline quality on InGaAs/InP substrates, however as for all heteroepitaxial systems, mechanical stress is an important issue which influences crystalline quality, film growth, and magnetic properties. One example is a magnetic anisotropy which depends on the thickness of the Half-Heusler layer [1].

We present a series of x-ray measurements on MBE-grown NiMnSb thin films from 15 to 120nm thickness. Reciprocal space mapping was performed using the six-circle-diffractometer at BW2, HASYLAB, Hamburg. Structural properties like the critical thickness for pseudomorphic growth, relaxation, and the poisson ratio of the Half-Heusler layers are discussed.

[1] A. Koveshnikov et al.: submitted to J. Appl. Phys. (2004).

O 38.9 Di 12:45 TU EB301

Characterization of the growth peculiarities of Physical Vapor Deposited CdS on Cu(In,Ga)Se_2 Thin Film Solar Cells Using Kelvin Probe Force Microscopy in Ultrahigh Vacuum — •Ferdinand Streicher, Marin Rusu, Christian A. Kaufmann, Axel Neisser, Susanne Siebentritt, Martha Ch. Lux-Steiner, and Thilo Glatzel — Hahn-Meitner-Institut Berlin, Glienicker Strasse 100, 14109 Berlin, GERMANY

High-efficiency thin-film solar cells based on Cu(In,Ga)Se_2 absorber material have been developed using CdS buffer layers deposited by chemical bath deposition (CBD). However, for industrial production, an inline vacuum deposition such as, e.g. physical vapour deposition (PVD) is preferred. This contribution reports on the preparation and characterization of highly-efficient ZnO/CdS/Cu(In,Ga)Se_2 solar cells with PVD-deposited CdS buffer layers. The PVD-CdS preparation conditions were optimized for the deposition of the CdS layers suitable for highly-efficient (14%, AM1.5, total area) thin film solar cells. Compared to the CBD deposition the ZnO/PVD-CdS/Cu(In,Ga)Se_2 solar cell devices show an increased short circuit current while open circuit voltage is decreased. The surface analysis of the CdS growth process with Kelvin probe force microscopy (KPFM) reveals, that the CdS deposition is retarded at the grainboundaries of the absorber which could be a reason for the observed device behavior.