HL 23 Interfaces/surfaces

Time: Tuesday 17:15–19:30 Room: BEY 154

HL 23.1 Tue 17:15 BEY 154

X-ray grazing incidence investigations of focused ion beam interactions with a Si and GaAs surfaces — •Jörg Grenzer[1], Ullrich Pietsch[2], Lothar Bischoff[1], and Matthias Posselt[1] — [1]Forschungszentrum Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, POB 51 01 19, D-01314 Dresden, Germany — [2]FB7 - Physik , Universität Siegen, 57068 Siegen, Germany

We report on the study of a two-dimensional dot lattice structures which was produced on GaAs and Si (001) substrates using a Ga^+ focused ion beam in normal incidence with a spot size of about $50nm$, an energy of $25keV$ and a dose of $10^{14}cm^{-2}$. The fabricated 2D-lattice structures consist of dots of almost circular shape ($2000nm^2$) and a period of $250x250nm^2$. We have investigated the interaction of the implanted ions with the host lattice as a function of the implantation conditions using grazing incidence diffraction at the ID10 and ID1 beam lines at the ESRF. The low-dose implantation creates interstitials and vacancies below the surface generating a weak displacement field resulting in a 2D periodical strain field in case of Si substrate. For the GaAs substrate we found a much more complex scattering pattern which depends on the in-plane orientation of the 2D dot lattice with respect to the substrate crystallographic orientation. A much stronger scattering contrast can be found if the 2D dot lattice misaligned by 14° degree. A simulation taking the interaction between the implanted ions and the host lattice into account shows an enhanced channelling of the ions into low-index crystallographic directions. Thus the dependence of the implantation damage profile on the crystalline structure influences the scattering patterns.

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Distribution of Co atoms on Si (100) investigated by high resolution Rutherford backscattering spectrometry. — •Saroj Prasad Dash, Dagmar Goll , and Heinz Dieter Carstanjen — Max- Planck- Institut für Metallforschung, Stuttgart, Germany

We have investigated the initial stages of the growth of Co on a Si (100) surface at room temperature. The structural evolutions and the material distribution on and below the surface for 0.08 ML to 3 ML Co coverage have been probed in situ by high resolution Rutherford back scattering spectrometry. We can clearly classify the coverage from 0.08 ML to 3 ML into two different regimes. For coverage of 0.08 ML to 1.09 ML we were able to observe Co atoms chemisorbed in the form of 2D islands on the surface and atoms on the sub-surfaces, showing higher bulk diffusivity than surface diffusivity of Co in Si. For coverage of 2 ML and 3 ML we could observe silicide-like phases on the surface. This gives a strong indication that for 2 ML and 3 ML coverage Si mass transport occurs from the substrate for silicide formation and lowers the surface free energy.

HL 23.3 Tue 17:45 BEY 154

Ripple morphology versus Ar+ implantation dose in silicon — •Souren Grigorian[1], Joerg Grenzer[2], and Ullrich Pietsch[1] — [1]University of Siegen, Institute of Physics, 57072 Siegen, Germany — [2]Forschungszentrum Rossendorf, Institut fuer Ionenstrahlphysik und Materialforschung, P.O. Box 510119, 01314 Dresden, Germany

Investigations of ripples morphology of Ar+ implanted silicon are presented. Particularly we have measured the degree of amorphization as a function of implantation dose by means of x-ray grazing amorphous scattering (GIAS). For perfect silicon crystals GIAS shows monotone decreasing background intensity versus the 2θ scattering angle. For implanted samples we find two broad peaks indicating short-range ordering of amorphous material changing with the penetration depth of probing x-ray. The appearance of embedded crystalline domains is indicated by additional sharp peaks on top of the amorphous scattering. 2θ- scans taken at different azimuthal angles of sample display strong anisotropy of amorphous scattering which only slightly changes with dose. Based on these results we suggest a model of dose-dependent amorphization. The strong damage of crystalline structure takes place along particular crystallographic directions and strongly reveal for low doses, before it becomes complete amorphous and mostly uniform at high doses of implantation. This mechanism can be used as a hint for the appearance of a ripples amorphous-crystalline interface found at these structures.

We would like to thank S. Hazra and T.K. Chini for research collaborations. This work was supported by the DST-DAAD India-Germany Collaborative Program.

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Quantitative characterization of a crystalline-amorphous interface by Q-HRTEM — •Karsten Thiel[1], Nikolai Borgardt[2], Boris Plikat[3], Tore Niermann[1], and Michael Seibt[1] — [1]IV. Physikalisches Institut der Universität Göttingen and SFB 602, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]permanent address: Moscow Institute of Electronic Technology, 103498 Moscow — [3]now at: Infineon Technologies AG, 93049 Regensburg

The atomic structure of the transition region between c-Si(111) and a-Ge as well as a-Si has been studied by means of Q-HRTEM. Our approach involves averaging of the images along the interface, and simulating them within the "averaged-projected-potential"approximation by multi-slice simulation. This includes the use of a 2D-distribution function $\rho(x, y)$ for the density of the atoms on the amorphous side and the well known atomic positions on the crystalline side.
$\rho(x, y)$ reveals lateral ordering close to the crystalline substrate in addition to a pronounced layering. The width of both transition regions could be estimated to ≈1.4nm and the bond-angle distribution in the 1st layer is determined as 11.5° for a-Ge and ≈2.1° for a-Si.
For the a-Ge sample, we also investigated the lateral variations of $\rho(x, y)$ and how far these changes are significant. It results, that there are no significant variations in the 1st atomic layer. This indicates homogenous properties for this layer on the scale of ≈23nm. In contrast, for the 2nd and 3rd layer we observe significant variations on a lateral scale of ≈10nm. We attribute these lateral variations to the response of the atomic network in the transition region on the volume misfit.

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The Role of Hydrogen in the Pre-epitaxial Cleaning of Silicon(100)-Surfaces — •Markus Schindler[1], Matthias Schmidt[1], Dorota Kułaga-Egger[1], Tanja Stimpel-Lindner[1], Jörg Schulze[1], Ignaz Eisele[1], and William Taylor[2] — [1]Universität der Bundeswehr München, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg — [2]Freescale Inc., Austin TX, USA

Due to the continous trend to smaller device dimensions in silicon microelectronics dopant diffusion and hence process temperature must be limited. In this work we investigate the minimum thermal budget to achieve contamination-free silicon surfaces prior to expitaxy in a commercial low pressure chemical vapour deposition (LPCVD)-system. Process parameters varied are temperature and oxygen partial pressure (steady-state-boundary). The samples are characterized with secondary-ion-mass-spectroscopy (SIMS) for oxygen- and carbon impurities. The presence of hydrogen in the growth enviroment leads to less stringent requirements for oxygen partial pressure and a complete removal of carbon impurities. For oxygen removal cleaning in inert gas ambient behaves similar to ultra-high-vacuum (UHV). The same reaction path seems to be valid for silicon substrate cleaning under hydrogen, argon and UHV conditions. We conclude that for low-temperature preepitaxial cleaning the oxygen partial pressure has to be lowered considerably in future LPCVD-systems.

HL 23.6 Tue 18:30 BEY 154

Structural and electronic properties of Si/SiOxNy interfaces — •Alberto Martinez-Limia, Rebecca Janisch, Philipp Pläntz, and Christian Radehaus — Institute for Electrical and Information Egineering, TU Chemnitz, 09112 Chemnitz, Germany

The incorporation of N into the gate oxide of metal-oxide-semiconductor devices is an extended practice in the present microelectronic technology. Improvements in the dielectric properties and suppression of dopant diffusion and material defects have been reported for this kind of materials.

To study structural an electronic properties of Si/SiOxNy interfaces we performed DFT calculations with CPMD and ABINIT codes. We generated several Si/SiOxNy model interfaces for low N concentrations. After structural optimization, the site projected density of states (DOS) was calculated for representative atoms of the system. With this information and using GW band gap results for the bulk phase of SiOxNy and Si we can evaluate valence and conduction band offsets of these systems. Changes of the DOS at the interface depending on concentration

and position of the N atoms on the SiOxNy phase are discussed.

HL 23.7 Tue 18:45 BEY 154

Removal of carbon and oxygen contaminants from silicon surfaces by atomic hydrogen — •Tanja Stimpel-Lindner[1], Markus Schindler[1], Günther Dollinger[2], Hermann Baumgärtner[1], and Ignaz Eisele[1] — [1]Institut für Physik, Fakultät für Elektrotechnik, Universität der Bundeswehr München, 85577 München-Neubiberg, Deutschland — [2]Institut für Angewandte Physik und Messtechnik, Fakultät für Luft- und Raumfahrttechnik, Universität der Bundeswehr München, 85577 München-Neubiberg, Deutschland

For the growth of nanostructures on silicon (Si), the previous cleaning of the substrate surface is an important step. Common processes for surface preparation in UHV involve temperatures up to 1200°C. For atomically sharp doping profiles and other innovative structures, this is far too high. Cleaning procedures at lower temperature regularly either leave carbon (C) and oxygen on the surface or produce a significant roughening of the surface which is also unwanted. In our work, a cleaning process using atomic hydrogen was developed. Starting from oxide-covered Si(100) after RCA-Cleaning or native silicon dioxide, both covered with carbon contaminations, the surfaces were exposed to atomic hydrogen which was generated by dissociative adsorption of hydrogen on a hot tantalum surface. With this new process, C can already be removed at substrate temperatures of about 500°C. Oxygen removal starts at slightly higher temperatures. The cleaning process was investigated in detail by XPS, AES and STM. These results will be compared with cleaning processes used by the semiconductor industry which also employ hydrogen.

HL 23.8 Tue 19:00 BEY 154

Electronic structure at Si-Insulator interfaces — •Rebecca Janisch, Alberto Martinez-Limia, and Christian V. Radehaus — Institute for Electrical and Information Engineering, Technical University Chemnitz, 09107 Chemnitz, Germany

Several materials systems are currently under consideration as potential alternatives to SiO$_2$ as the gate dielectric material for complementary metal-oxide-semiconductor (CMOS) technology. One of the main challenges for the alternative high-k dielectric are the advantageous structural features of the Si-SiO$_2$ interface. Pseudobinary alloys of SiO$_2$ and the oxides of the group-IV transition metals Ti, Zr, and Hf are currently considered to be the most promising candidates that combine the outstanding structural features of the former with excellent dielectric properties of the latter.

To study the electronic properties of Si-high-k interfaces, we performed ab initio calculations employing the ABINIT and the CPMD electronic structure code. In a first step we constructed a model Si-SiO$_2$ interface. After structural optimization we calculated site-projected density of states (DOS) for representative atoms in the supercell. From these we were able to derive information about band-offsets and the density of interface states. Starting with the relaxed structure of the Si-SiO$_2$ interface we then substituted selected Si atoms in the SiO$_2$ slab with Ti or Zr respectively. We currently investigate the preferred position of the substituting atom, its influence on the bulk and interface structure, as well as the resulting changes in the electronic structure at the interface. We will discuss the results of this ongoing work in this presentation.

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Ab initio Calculation of Structural and Electronic Properties of Interfaces between Ionic Compounds: PbTe(rs)/CdTe(zb) — •Roman Leitsmann, L.E. Ramos, and F. Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The structural and electronic properties of {100} and {110} PbTe(rs)/CdTe(zb) interfaces are investigated by means of an ab initio pseudopotential method. Both materials have a strong polar character. The repeated slab approximation to model the interfaces gives rise to resulting dipole moments in the {100} case. Therefore an artificial potential is induced due to the periodic boundary conditions of the super cell approach[1]. We have developed a new scheme to calculate the interface energies and the projected band structures of such systems. First results will be presented and compared with recent experimental observations.

[1] Jörg Neugebauer and Matthias Scheffler, Phys. Rev. B 46, 16067 (1992)