X-ray grazing incidence investigations of focused ion beam interactions with a Si and GaAs surfaces 

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We report on the study of a two-dimensional dot lattice structures which were produced on GaAs and Si (001) substrates using a Ga⁺ focused ion beam in normal incidence with a spot size of about 2.0 \(\mu\)m. We used an energy of 25keV and a dose of \(10^9\) cm⁻². The fabricated 2D-lattice structures consist of dots of almost circular shape (2000 nm) and a period of 250x250 nm². 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 DI10 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°. A simulation taking into account the interaction between the implanted ions and the host lattice into account of an enhanced channeling of the ions into low-index crystallographic directions. Thus the dependence of the implantation damage profile on the crystalline structure influences the scattering patterns.

**Distribution of Co atoms on Si (100) investigated by high resolution Rutherford backscattering spectrometry.**  

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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 (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 (100) surface. The structural evolutions and the material distribution on and below the surface for 0.08 ML to 3 ML Co (100) surface. The structural evolutions and the material distribution on and below the surface for 0.08 ML to 3 ML Co (100) surface. The structural evolutions and the material distribution on and below the surface for 0.08 ML to 3 ML Co (100) surface.

**Ripple morphology versus Ar⁺ implantation dose in silicon.**  

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Investigations of the ripple 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 (GAS). For perfect silicon crystals GAS shows monotonous decreasing background intensity versus the 2θ scattering angle. For implanted samples we find two broad peaks indicating short-range ordering of amorphous material and 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. 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.

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Due to the continuous 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 epitaxy 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 environment leads to less stringent requirements for oxygen partial pressure and a complete removal of carbon impurities. For oxygen removal cleaning in inert gas ambient below 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.

**Structural and electronic properties of Si/SiOxNy interfaces.**  

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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.

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Removal of carbon and oxygen contaminants from silicon surfaces by atomic hydrogen — Tanja Stimpel-Lindner, Markus Schindler, Günther Dollinger, Hermann Baumgartner, and Ignaz Eisele — Institut für Physik, Fakultät für Elektrotechnik, Universität der Bundeswehr München, 85577 München-Neubiberg, Deutschland — 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.

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.

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.