

HL 26: Interfaces and Surfaces

Time: Monday 16:00–17:45

Location: POT 06

HL 26.1 Mon 16:00 POT 06

Focused Ion Beam Structuring of Ag Nanowires with Single Grain Boundaries for Electromigration Experiments —

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Electromigration is decided by the balance of two opposing forces. On one hand the wind force acts via the momentum transfer from the conduction electrons to the atoms, on the other hand the so-called direct force arises from the electric field. Structural features have been shown to change the balance of the forces. Whereas the wind force dominates the electromigration in poly-crystalline Ag and Au nanowires [1], in single-crystalline Ag nanowires, the direct force drives the electromigration opposite to the direction of electron movement [2]. Here we present a new approach to study the electromigration in Ag nanowires with a single grain boundary. Focused ion beam (FIB) is used to structure wires from epitaxially grown Ag islands with two different crystallographic orientations, Ag(001) and Ag(111). While FIB structuring of Ag wires has promising prospects, there are some downsides as well. The issues, e.g. doping of the Si substrate and amorphisation, and possible solutions will be discussed. First electromigration experiments will be presented.

[1] B. Stahlmecke and G. Dumpich, *JPCM* **19** (2007) 046210

[2] B. Stahlmecke et al. *APL* **88** (2006) 053122

HL 26.2 Mon 16:15 POT 06

Time Scaling of Silver Nano-Crystal Growth at the Interface of Silver Thick Film Electrodes on n-Type Silicon —

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The interface of silver thick film contacts on n-type silicon features nanoscale silver crystals. They carry the current across such interfaces and hence govern the contact resistance which is a main performance limiting parameter for semiconductor devices. The silver crystals form in pits on the silicon surface at the interface during a high temperature step. In earlier studies we simulated the growth of these pits by considering the probability of removing a silicon surface atom in dependence of its bond energy. In the present work we present a method for introducing a quantitative time scaling for these simulations. This method leads to good quantitative agreement between simulated and experimental data. It enables the prediction of pit formation and hence silver crystal growth for arbitrary process parameters like temperature and duration during silver thick film contact formation on n-type silicon.

HL 26.3 Mon 16:30 POT 06

Nanowire-metal hybrid structures: the influence of the deposition technique on the optical properties —

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ZnO nanowires (NWs) have drawn widespread attention for their potential use in many optical devices. Recently, surface plasmon resonances of metal nanoparticles (NPs) have been used to increase the quantum efficiency of near-band-edge (NBE) spontaneous emission of these nanowires. However, we observed that the metal NPs deposition process itself significantly influences the optical properties. We investigated the time-integrated and time-resolved photoluminescence (PL) properties of ZnO NWs coated with Au, Ag and Pt NPs which were deposited by DC sputtering in Ar plasma. The influence of the sputtering process was determined by performing the same sputtering treatment while shielding the sample to avoid metal deposition. A strong enhancement of the NBE emission and a quenching of the deep-level emission were observed in all cases. Time-resolved spectroscopy showed a reduction of the radiative lifetime in all samples irrespective of size and kind of metal NPs. PL studies at 4 K revealed a strong hydrogen-donor-bound-exciton line indicating unintentional incorporation of hydrogen. The results can be explained by considering the passivation of deep centers by hydrogen and the introduction of a large amount of hydrogen donors.

HL 26.4 Mon 16:45 POT 06

Lithium Diffusion at Silicon Surfaces —

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Lithium-ion batteries are in common use in a large number of modern electrical appliances. In the quest for ever higher storage capacities new electrode materials are needed which will eventually replace the commonly used graphite anodes. Silicon is a promising candidate due to its enormous storage capacity for lithium but suffers from a large density difference between the lithium containing and lithium free phase. Nano-structured materials (particles, wires etc.) promise to remedy this problem. Transport processes at the surface of silicon anode surfaces are therefore of keen interest.

We have studied the diffusion of lithium into silicon under UHV conditions and at low temperatures (150-180 K) using Auger and X-ray photoelectron spectroscopy. Thin layers of lithium were deposited on pristine H-passivated Si(001) and oxygen modified surfaces at a temperature (120 K) that effectively suppresses the diffusion, although a thin layer of silicide forms at the interface right away. At sufficiently high temperatures diffusion of lithium into the bulk sets in, which can be monitored through the attenuation of the silicon signal underneath the metallic lithium film. The formation of surface silicide is a thermally activated process with an activation energy of 0.49 eV.

HL 26.5 Mon 17:00 POT 06

Adsorption of Methanol on Lithium niobate (0001) —

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Lithium niobate (LN) is a ferroelectric material with a huge range of applications. While the bulk properties of LN are exploited in optical and acoustic devices, the physics on the different oriented surfaces allows the realization of molecular detectors and other devices at nanoscale level. Temperature programmed desorption measurements of polar molecules, such as Water, Methanol [1], and 2-Propanol [2], on the (0001) LN surfaces show stronger adsorption of these molecules on the positive surface. The mechanisms behind the bonding are still not clear. Recently, structural models for the negative and positive (0001) surface of LN have been proposed on the basis of Density Functional Theory (DFT) calculations. Here, we investigate the behavior of Methanol on the LN surfaces by means of DFT in the Generalized Gradient approximation (GGA). As a first step, we calculate the potential energy surface (PES) for both orientations. We find the preferred position of an adsorption of Methanol near the Oxygen atoms on the positive or near the Lithium atoms on the negative surface, respectively and a bonding-energy difference of about 0.5 eV between the two sites. Also, we investigate the possibility of a dissociation of the molecule on the LN surfaces.

[1] J. Garra *et al.*, *Surface Science* **603** (2009) 1106 - 1114

[2] Y. Yun *et al.*, *J. Phys. Chem. C* **111** (2007) 13951-13956

HL 26.6 Mon 17:15 POT 06

Photoemission spectroscopy studies of SrTiO₃ and its interface to gold —

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Motivated by applications of strontium titanate (SrTiO₃, STO) in non-volatile memory devices we studied the surface of STO by means of x-ray and ultra violet photoemission spectroscopy. The focus of the analysis was purity, doping and the annealing time. It could be demonstrated that a surface contamination layer consisting of carbonates and hydroxides exists on surfaces prepared under ambient conditions. In addition, the interface between STO and gold was investigated. We show that there is a weak interaction of these materials, however a Schottky-type Au/SrTiO₃ junction is formed. Finally the work function of all STO samples was determined. The work function depends on the modification of the STO surface. This fact should be considered for the formation of such a Schottky-type junction.

HL 26.7 Mon 17:30 POT 06

Contributions to the *in situ* RAS signal of MOVPE prepared GaP/Si(100) — ●OLIVER SUPPLIE, HENNING DÖSCHER, SEBASTIAN BRÜCKNER, ANJA DOBRICH, PETER KLEINSCHMIDT, and THOMAS HANNAPPEL — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

High efficient opto-electronic devices based on III-V/Si(100) heterostructures require low defect densities within the active material. Reflection Anisotropy Spectroscopy (RAS) signals from optically isotropic crystals can be related to surfaces, interfaces or defects within the bulk and allow for *in situ* characterization during metal organic vapor phase epitaxy (MOVPE). The (1×2)-like surface reconstruction of P-rich prepared GaP(100) yields a characteristic RA spectrum [1].

Deviations in the RA spectra of thin GaP/Si(100) films of different thicknesses can originate from (1) internal reflections, i.e. interference, (2) the pure surface anisotropy, (3) anti phase disorder induced at the heterointerface, (4) GaP bulk anisotropies, and (5) a possibly anisotropic GaP/Si(100) interface itself. Those contributions can be separated by optical models [2]. The peak intensities of the pure surface signal allow for improved *in situ* quantification of the anti phase domain content at the GaP/Si(100) surface and is in agreement with the GaP(100) surface anisotropy. Neglecting GaP-bulk contributions, an interface anisotropy consistent for different GaP film thicknesses can be extracted.

[1] H. Döscher et al. JAP **107** (2010) 123523. [2] T. Yasuda. TSF **313** (1998) 544, O. Hunderi et al. TSF **472** (2005) 261.