Electromigration is decided by the balance of two opposing forces. On one hand, the force acts via the forced motion of 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 polycrystalline 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 when considering the FIB process itself significantly influences the optical properties. 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.

Lithium-ion batteries are in common use in a large number of modern electronic 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.

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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 strong 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 prefered 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.

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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.