

MS12.01.05 STRUCTURE ANALYSIS OF CoSi₂/Si_{1-x}Gex/Si(001) INTERFACES. M. Rodewald, TH Darmstadt, FB21, FG Strukturforschung, Petersenstr. 20, D64287 Darmstadt, Germany

In the last decade silicide growth and silicide/silicon interfaces have become of interest in solid state science because epitaxial metal silicides are a promising material for novel micro-electronic devices like the metal-base and the permeable base transistors.

In the present investigation monocrystalline (001) oriented films of CoSi₂ have been formed on Si_{1-x}Gex/Silicon(001) heterostructures with Ge-contents up to 25at.% by molecular beam epitaxy (1). The atomic structure of the CoSi₂/Si_{1-x}Gex interface has been investigated by high resolution electron microscopy (HREM) combined with image contrast simulations.

A domain-like structure is observed consisting of areas with different interface structure interconnected with steps. Two different atomic structure models for the different interface areas have been found by comparison of simulated and experimental images. In the first model evidence for a 2x1 (and 1x2) interface reconstruction was found. This interface reconstruction is different from the already known interface reconstruction of CoSi₂/Si(001) interfaces (2, 3). In the second model the Co-atoms are 6fold coordinated at the interface and the tetrahedral coordination of the silicon atoms is everywhere maintained. This model is well known from CoSi₂/Si(001) interfaces.

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MS12.01.06 ORDERED STRUCTURES AT THE METAL ELECTRODESOLUTION INTERFACE. C. A. Lucas, N. M. Markovic and P. N. Ross. Materials Sciences Division, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720

Unraveling the atomic structure at the metal-electrode/solution interface presents a great challenge to the experimentalist due to its inherently complex nature. X-ray diffraction is an ideal tool for studying this structure and the related surface electrochemical phenomena, as the penetrating nature of x-ray radiation allows *in situ* study of the metal surface. In contrast to studies of adsorbate systems in ultrahigh-vacuum, adsorbate structures at the electrode surface are complicated by the range of possible adsorbing species in solution. We have performed a series of experiments with Pt(hkl) electrodes to determine the role of anion adsorption in surface reconstruction, surface relaxation and during the underpotential deposition (UPD) of metals. Information is obtained via measurement of the in-plane diffraction satellites due to ordered 2D adlayers and by measurement of the 'crystal truncation rods' (CTR's) to relate the positions of the surface atoms with respect to the bulk Pt lattice. Monitoring the scattered intensity at selected reciprocal lattice points as a function of the electrode potential is key to understanding the sequence of adsorbed structures. Interpretation of the x-ray results is aided by the use of anomalous scattering methods to obtain chemical sensitivity in deriving structural models.

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MS12.01.07 SCALING OF SUBMONOLAYER Cu ISLANDS GROWN ON Cu(110). D.A. Walko, K.L. Whiteaker, and I.K. Robinson, University of Illinois, Urbana, IL 61801

The structure and properties of a thin film are often determined by the growth conditions as the first monolayer is deposited. We have studied the influence of an anisotropic substrate on the nucleation, growth, and coalescence of homoepitaxial islands. Surface x-ray diffraction was used *in situ* to study submonolayer deposition of Cu on Cu(110). After deposition, we found diffuse scattering near the out-of-phase condition featuring an elliptical ring, which is due to the anisotropic island morphologies. The major and minor axes of the ellipse are proportional to the island densities (or inversely proportional to the island spacing) in the in-plane [001] and [1,-1,0] directions respectively. The density of islands in each of these directions scales with deposition rate and with substrate temperature. However, the scaling results are not well-described by mean-field rate equation formulations which fail to account for the full complexity of the fcc(110) surface. Evidence for a transition from one to two-dimensional island growth is seen at $T \sim 208$ K.

PS12.01.08 3-D STRUCTURAL ANALYSIS OF Ag/Si(111) INTERFACES BY X-RAY DIFFRACTION. R. D. Aburano, Hawoong Hong, J. M. Roesler, K.-S. Chung, H. Chen and T.-C. Chiang, University of Illinois, and P. Zschack, ORISE.

The interface of the "prototypical nonreactive" Ag/Si(111) system exhibits different structures depending upon the interfacial preparation. Room temperature deposition of a Ag film on a clean Si(111)-(7x7) surface results in a Ag-modified (7x7) structure at the interface. This structure transforms to a bulk-like (1x1) structure when annealed above 200°C. This temperature is characteristic for the formation of the (orb) on Si(111). This (3x3)R 30°-Ag reconstruction is also not retained at the interface even when it is buried under a room temperature deposited Ag film. Crystal truncation rod analysis of the Ag-modified (7x7) and (1x1) structures revealed the preservation of the Si stacking fault in the former and a Ag-Si mixed layer at the interface in the latter. These results may provide some insight into the observed Shottky barrier height difference for these two interfaces.

PS12.01.09 ANALYSIS OF IN-PLANE STRUCTURES OF THE As-DEPOSITED Si SURFACES USING GRAZING-ANGLE X-RAY STANDING WAVES. O. Sakata, S. Kumano, N. Matsuki, Y. Tanaka, A. M. Nikolaenko, H. Hashizume, Res. Lab. Eng. Mater., Tokyo Institute of Technology, Nagatsuta, Midori, Yokohama 226, Japan

We applied grazing-angle X-ray standing waves to a Si(111):As 1x1 surface to determine the in-plane position and order of As atoms under UHV condition (Sakata & Hashizume (1995)). As *K* emission profiles showed As atoms located in the threefold coordinated sites of the bulklike Si(111) surface with little disorder. The displacement is smaller than 2% of the *d* spacing of the (2 20) planes and the coherent fraction is higher than 80%. This technique has now been applied to the Si(100):As surface. The substrate Si surface was cut 4° off the (100) plane to favor the 2x1 structure over the 1x2 structure. The As emission data collected in the vicinities of the 022 and 0 2 2 Bragg peaks under UHV condition at the Photon Factory synchrotron source were fit to a model including parameters for the area ratio of the 2x1 and 1x2 domains (M_2 , M_1) and the normalized As-As dimer bondlength ($2l$). The fits determined η parameters defined by $\eta = M_i + M_j \cos(2\pi l)$ ($i, j = 1, 2$). Solving the equations using the values of $\eta_1 = 0.42$ and $\eta_2 = 0.066$ obtained from the fit under the assumption $l = 0.664$, corresponding to 2.55 Å, gave $M_1 = 0.38$ and $M_2 = 0.62$. This indicates a highly ordered surface with no As atoms in random positions.

Sakata, O. and Hashizume, H. (1995) Acta Cryst. A51, 375-384.