DS 11: Layer Growth: Evolution of Structure and Simulation

Time: Tuesday 14:00–16:00 Location: GER 37

DS 11.1 Tue 14:00 GER 37

Material dependent smoothing of rippled surfaces — •Johanna Röder and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

Any kind of processing of materials like thin film deposition, ion beam treatment or polishing often creates structures, which have lateral length scales of 20-200 nm. For many applications, like optical mirrors or thin multilayer structures, it is important to avoid roughnesses in these dimensions. Up to now a lot of experimental and theoretical work has been done to investigate the roughness evolution during film growth on a smooth substrate. Another approach is the investigation of the growth of films deposited on already rough surfaces, where smoothing mechanisms influence the evolution of the surface and can be analysed more easily. In this contribution, the successive smoothing of artificially created rough surfaces has been studied by atomic force microscopy. Therefore periodic structured Si(100) surfaces (height of 4,5nm, period of 55nm) produced by sputter erosion were chosen as model system and systematically covered by thin layers of different material classes like oxides (ZrO_2), simple carbides (C) and polymers (PC). The results were discussed with respect to the dominating smoothing mechanisms that occur during deposition. The scaling behaviour of the roughness evolution was investigated in Fourier space using power spectral densities (PSD). The three material classes will be compared and the differences during the smoothing process discussed. All samples were deposited by pulsed laser deposition.

DS 11.2 Tue 14:15 GER 37

Stacking fault suppression in ion assisted growth of Ir on Ir(111) — •Sebastian Bleikamp and Thomas Michely — Institute of Physics 2, University of Cologne, Germany

Due to their low energy, stacking faults are among the most frequent defects in thin films.

In homoepitaxy of Ir on Ir(111) around room temperature, stacking faults are formed in large numbers, which propagate through the growing film, causing extended defect structures. Eventually thin Ir films become heavily twinned and grow rough due to the twin associated defects.

Here we present kinetic strategies for the avoidance of stacking fault propagation and defect structure formation based on ion assistance. Ir is evaporated with ion assistance of 100eV Ar^+ ions at normal incidence with an ion to atom arrival ratio of R=1:2 or with ion assistance of 500eV Ar^+ ions incident at an angle of 85° with respect to the surface normal with R=1:10. Based on scanning tunneling microscopy investigations we find that this treatment transfers the growth mode to layer-by-layer growth and no twin crystallites are formed. The result is backed up by low energy electron diffraction measurements. Annealing shows that a significant amount of noble gas is incorporated in the films during growth. Gas incorporation could be avoided if the necessary energy could be supplied to the Ir atoms themselves.

Analysis of the atomic processes involved indicates that the key action of the ions is to destroy the defect structures stabilizing the faults, rather than to suppress fault nucleation.

DS 11.3 Tue 14:30 GER 37

Ion induced Burying Effect of Au Nanoparticles on SiO_2: Influence of Sputtering — A. Klimmer[1], M. Trautvetter[1], B. Kuerbanjiang[2], •P. Ziemann[1], J. Biskupek[2], and U. Kaiser[2] — [1]Universität Ulm, Institut für Festkörperphysik, D-89069 Ulm — [2]Universität Ulm, ZE Elektronenmikroskopie, D-89069 Ulm

Ordered arrays of spherical Au nanoparticles (NP) exhibiting narrow size distributions were fabricated on top of SiO_2 substrates applying a micellar preparation technique [1]. Ion irradiating such NP arrays of different starting diameters with 200 keV Ar^+ and Xe^+, respectively, leads to a burying effect until the NP are completely covered. Combining HRTEM data with AFM height measurements delivering the necessary statistics allows a quantitative analysis of the phenomenon. It will be demonstrated that in addition to the necessary thermodynamic driving forces related to an ion induced enhancement of the substrate viscosity and to the various surface and interface energies [2], sputtering of the NP with a size-dependent sputter yield has to be included in the description of the experimental results in order to improve agreement.

[1] Micellar Nanoreactors: Preparation and Characterization of Hexagonally Ordered Arrays of Metallic Nanodots, G. Kästle at al., Adv. Funct. Mater. 13, 853 (2003). [2] Burrowing of Pt nanoparticles into SiO_2 during ion-beam irradiation, X. Hu, D. G. Cahill, R. S. Averback, J. Appl. Phys. 92, 3995 (2002).

DS 11.4 Tue 14:45 GER 37

Basics of the atomic layer deposition of HfO_2 onto Si/SiO_2 substrates: *in-situ* investigations with XPS, XAS and UHV-AFM — •Massimo Tallarida, Konstantin Karavaev, Krzysztof Kolanek, and Dieter Schmeisser — Brandenburgische Technische Universität, LS Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee, 17, 03046, Cottbus, Germany

We developed a reactor for investigating *in-situ* the atomic layer deposition (ALD) of HfO_2. X-ray photoelectron and X-ray absorption spectra were collected after each ALD cycle using synchrotron radiation at the beamline U49-2/PGM2 - BESSY II, Berlin. The morphology of the substrate and thin film surfaces was investigated after each ALD cycle with an UHV-AFM microscopy attached to the ALD reactor. We studied the ALD on differently prepared substrates, at different substrate temperatures, and using different Hf-precursors ($HfCl_4$, TEMAHf, TDMAHf). We observed the evolution of the $Si/SiO_2/HfO_2$ system during the formation of the first three Hf-oxide layers [1]; we detected the incorporation of Cl into the Hf-oxide films and proposed a mechanism responsible for the Cl contamination [2]; we found evidence of the interfacial-SiO_2 growth during the initial ALD cycles and of dipole formation at the HfO_2/SiO_2 interface. In this contribution we illustrate the basics of the technique used, and discuss the physical-chemical properties of ALD on the basis of the experimental results.
[1] M. Tallarida, K. Karavaev, and D. Schmeisser, J. Appl. Phys. **104**, 064116 (2008); **[2]** M. Tallarida, K. Karavaev, and D. Schmeisser, J. Vac. Sci. Technol. B, accepted for publication.

DS 11.5 Tue 15:00 GER 37

Evolution of the interfacial layer during the atomic layer deposition of HfO_2 on Si/SiO_2 substrates — •Konstantin Karavaev, Massimo Tallarida, and Dieter Schmeisser — Brandenburgische Technische Universität, LS Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee, 17, 03046, Cottbus, Germany

We studied the formation of the interfacial layer in the $Si/SiO_2/HfO_2$ system using the *in-situ* Atomic Layer Deposition (ALD) reactor developed in our group [1,2]. We measured the X-ray photoelectron and X-ray absorption spectra with synchrotron radiation at the beamline U49-2/PGM2-BESSY II. The ALD growth was obtained using different Hf-precursors ($HfCl_4$,TEMAHf and TDMAHf) on various prepared substrates at different temperatures. The investigation was carried out *in-situ* giving the possibility to determine the properties of the grown film after every ALD cycle without breaking the vacuum. We observed the evolution of the $Si/SiO_2/HfO_2$ system during the formation of first three Hf-oxide layers, detecting the interfacial growth of SiO_2 during the initial ALD cycles from the XPS spectra of Si2p. We discuss how the interfacial layer growth depends on the various ALD parameters.
[1] M. Tallarida, K. Karavaev, and D. Schmeisser, J. Appl. Phys. **104**, 064116 (2008); **[2]** M. Tallarida, K. Karavaev, and D. Schmeisser, J. Vac. Sci. Technol. B, accepted for publication.

DS 11.6 Tue 15:15 GER 37

***In-situ* investigations of the atomic layer deposition of HfO_2 with UHV/AFM** — •Krzysztof Kolanek, Konstantin Karavaev, Massimo Tallarida, and Dieter Schmeisser — Brandenburgische Technische Universität, LS Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee, 17, 03046, Cottbus, Germany

We studied *in-situ* the atomic layer deposition (ALD) of HfO_2 with ultra high vacuum (UHV) atomic force microscope (AFM), using the ALD reactor developed by our group [1, 2]. The reactor was attached to the Omicron Large Sample-UHV/AFM system in the AFM-Lab of the Angewandte Physik-Sensorik chair at the BTU-Cottbus. We investigated different $Si(001)/SiO_2$ substrates and surface preparation techniques performed before the ALD process. After each ALD cycle (using TDMAHf and H_2O as precursors), we studied the influence of the HfO_2 growth on the root mean square (RMS) roughness; the sur-

face fractal dimension and the height histogram: the surface skewness and kurtosis. We focused on the influence of the substrate temperature on the surface topography during the ALD. The *in-situ* studies of the ALD process with the UHV/AFM system correlated with the experiments performed with photoelectron spectroscopy can be used for understanding the fundamental properties of the ALD of HfO_2 on Si(001).

[**1**] M. Tallarida, K. Karavaev, and D. Schmeisser, J. Appl. Phys. **104**, 064116 (2008); [**2**] M. Tallarida, K. Karavaev, and D. Schmeisser, J. Vac. Sci. Technol. B, accepted for publication.

DS 11.7 Tue 15:30 GER 37

Pattern Formation in Langmuir-Blodgett Transfer Systems — •Michael Hubert Köpf and Rudolf Friedrich — Institut für Theoretische Physik, Wilhelm-Klemm-Str. 9, 48149 Münster

Self-organized regular patterns have been observed in experiments when phospholipid monolayers were transferred onto solid substrates via Langmuir-Blodgett technique. These patterns consist of broad areas of lipid in the liquid-expanded phase divided by equidistant groove-like liquid-condensed areas.

We present a theoretical investigation of the mechanism behind these phenomena. In our approach two coupled equations, one for the surfactant and one for the subphase, serve as a theoretical model of the experimental setup. The observed pattern formation occurs, when the monolayer on the subphase is close to the so-called main transition, the phase transition between the liquid-expanded and the liquid-condensed phase. We expect this transition to play a key role in the process of pattern formation. Within our framework, a transition of the surfactant phase directly affects the fluid by a change of surface tension. The interplay of surface thermodynamics and film evolution then builds up oscillations which finally lead to the observed structure. Linear stability analysis is applied in order to trace the instabilities behind the pattern formation and the dynamics of the system are investigated by means of numerical simulation.

DS 11.8 Tue 15:45 GER 37

Wachstum dünner $Ni_{63}Al_{37}$-Legierungsschichten auf Cu(001) — •Wolfgang Donner[1] und Noureddine Anibou[2] — [1]Fachgebiet Materialwissenschaften, Strukturforschung, Technische Universität Darmstadt — [2]XStream Systems Inc., Sebastian (FL), USA

Wir untersuchen den Einfluß epitaktischer Spannungen auf die Phasenstabilität dünner NiAl Schichten, die mittels Kathodenstrahlzerstäubung auf Kupfer Pufferschichten auf Silizium aufgewachsen wurden. Mit Hilfe systematischer Messungen an Proben unterschiedlicher Dicke und unter Nutzung der Tiefenselektivität von Röntgenbeugung unter streifendem Einfall kommen wir zu dem Schluß, daß die wachsenden Schichten eine Reihe struktureller Änderungen als Funktion der Schichtdicke erleiden. Die strukturelle Phase, die sich zuerst auf der Cu(001) Oberfläche bildet, stimmt nicht mit der von der mittleren Zusammensetzung her erwarteten Struktur überein. Vielmehr bildet sich zunächst die Phase, die die geringste Fehlanpassung zum Substrat aufweist. Dieser Effekt ("composition pinning") ist von kovalent gebundenen Halbleiterschichten her bekannt, unter Metallschichten aber selten.