

O 19 Nanostrukturen II

Zeit: Samstag 10:45–13:00

Raum: TU EB420

O 19.1 Sa 10:45 TU EB420

First Principles Simulations of Ice Nucleation at Metal Surfaces — ●ANGELOS MICHAELIDES and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195, Berlin

Ice nucleation at solid surfaces is of relevance to countless scientific and technological processes. In particular the nucleation of ice nano-crystals on metal surfaces is often a key first step in cloud formation and corrosion [1]. Yet unfortunately this remains one of the most poorly understood natural phenomena; severely lacking in atomic level understanding. Here, we discuss detailed density functional theory studies aimed at putting our understanding of ice nucleation at metals on a much firmer footing. Specifically the properties of H₂O hexamers - the smallest 'building blocks' of ice - adsorbed on a number of close-packed transition metal surfaces have been examined. We find that the competing influences of substrate reactivity and hexamer-substrate epitaxial mismatch conspire to yield a rich variety of (novel) hexameric ice structures, some of which have been observed by recent scanning tunnelling microscopy experiments [2]. [1] H.R. Pruppacher and J.D. Klett, *Microphysics of Clouds and Precipitation*, (Kluwer, Dordrecht, 2003)

[2] K. Morgenstern, *et al.*, (To be published).

O 19.2 Sa 11:00 TU EB420

Theoretical analysis of quantum-size effects of Pb(100) films – the role of symmetry and implications for “electronic growth” — ●DENGKE YU and MATTHIAS SCHEFFLER — Fritz Haber Institut, Berlin

We performed detailed density-functional theory studies of lead films as function of thickness. In particular we will discuss in this talk the total energies, bandstructures, workfunctions, and surface relaxations. The results for Pb(100) exhibit noticeable oscillation with thickness which are ruled by quantum well states of different character. Their interplay gives rise to an interesting behavior that goes beyond the standard free-electron description of quantum-size effect. Consequences for “electronic growth”, i.e. for an enhanced stability of certain film thicknesses are discussed. We also compare our finding in Pb(100) with other lead surface orientations.

O 19.3 Sa 11:15 TU EB420

Ab initio study of vicinal surfaces: electronic confinement, magnetic wires and adsorbate interactions — ●A.L. KLAVSYUK¹, V.S. STEPANYUK¹, W. HERGERT², and P. BRUNO¹ — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — ²Fachbereich Physik, Martin-Luther-Universität, Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany

Electronic structure of Cu(554) is studied using the density functional theory and the SKKR Green's function method. The band dispersion is presented. We compare our results for Cu(554) and Cu(111). The confinement of surface-state electrons near steps is discussed. The short and long-range electronic interactions between magnetic adatoms near steps and on the terrace are calculated. The effect of the electronic confinement on the adsorbate-adsorbate interaction is demonstrated. We study the influence of the decoration of step edges with Fe monoatomic rows on the behavior of surface-state electrons confined between regularly arranged steps. Confinement of unoccupied states in monoatomic chains is discussed. The atomic relaxations near steps on Cu(554) and Fe/Cu(554) are determined performing atomic-scale simulations with the ab initio based interatomic potentials.

O 19.4 Sa 11:30 TU EB420

Talbot effect on 2D colloidal crystals — ●MANUEL GONÇALVES and OTHMAR MARTI — University of Ulm - Dept. of Experimental Physics, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

The Talbot effect occurs when a two-dimensional periodic structure is illuminated by a planar wavefront. The standard theoretical explanation of this effect is based on Fresnel diffraction and on the paraxial approximation. The assumptions used for the Fresnel diffraction and the paraxial approximation do not apply for structures with lattice constants comparable to the wavelength. Colloidal crystals of spheres with a diameter of few micrometers have been produced. The 2D crystals, under planar illumination of laser light, produce self-images. The distance between the crystal and the self-image depends on the symmetry of the lattice, on the

wavelength and on the lattice constant. The experimental results have been compared with simulations based on the diffraction at an array of small apertures, using Rayleigh-Sommerfeld diffraction integrals without any approximations. The experimental data shows that colloidal crystals can be used as Talbot illuminators for distances of several tenths of μm .

O 19.5 Sa 11:45 TU EB420

Ioneninduzierte Defektstrukturen auf Oberflächen — ●THORSTEN PETERS¹, HENNING LEBIUS² und MARIKA SCHLEBERGER¹ — ¹Universität Duisburg-Essen, Fachbereich Physik, 45117 Essen — ²CIRIL GANIL, rue Claude Bloch, BP 5133, 14070 Caen, Cedex 5, France

Hochgeladene Ionen bieten die Möglichkeit, nicht nur über ihre kinetische, sondern auch über ihre potentielle Energie sehr hohe Energiedichten auf Oberflächen zu erzielen (bis zu $10^{14}\text{W}/\text{cm}^2$) und dort bleibende Defekte zu verursachen. Wir haben untersucht, inwiefern das Einbringen hoher potentieller Energien auf Isolator- (SrTiO₃, TiO₂, SiO₂ und Al₂O₃) und Halbleiteroberflächen (Si) zu Defekten in der Oberflächenmorphologie führt. Bestrahlt wurden die Proben mit ³⁶S¹⁵⁺-, ²⁰⁸Pb²³⁺-, ¹²⁹Xe¹⁵⁺ und ¹²⁹Xe²⁹⁺- Ionen mit Energien zwischen 270 keV und 410 MeV. Untersucht wurde jeweils die Oberflächenbeschaffenheit mittels Rasterkraftmikroskopie, sowohl an Luft als auch *in situ* direkt nach Präparation und Bestrahlung. Es konnte gezeigt werden, dass sich nur für bestimmte Projektil-Oberflächen-Kombinationen einzelne Defekte auf den Oberflächen in Form von hügelartigen Erhebungen ausbilden. Der quantitative Zusammenhang zwischen dem Ladungszustand der Projektile und der Anzahl, Form und Abmessungen der Defekte soll in zukünftigen Experimenten näher untersucht werden.

O 19.6 Sa 12:00 TU EB420

Grazing incidence Ar⁺ ion induced creation and azimuth dependent evolution of nanogrooves on Cu(001) — ●HERBERT WORMEESTER, MICHAEL OVSYANKO, GEOIGIANA STOIAN, and BENE POELSEMA — MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Grazing incidence 800 eV Ar⁺ sputtering on a Cu(001) surface leads to the formation of nanogrooves in which only 3 layers are involved. With high resolution LEED we found that initially the distance between the nanogrooves L depends linearly on the sputter time: $L=L_0+St$. Both the initial average distance L₀ and a separation rate S depends on temperature. For sputtering along the [110] and [100] azimuths, a similar L₀ is found while a higher slope is observed along [100]. For increased sputter time, L clearly saturates for sputtering along the [100]. Annealing experiments of initially created grooves show a similar separation rate S, indicating that this behaviour does not originate from the ion sputtering. The temporal evolution and observed saturation of the distance between the nanogrooves along both the [100] and [110] azimuth will be discussed.

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Pattern defects and their effect on roughness in ion bombardement induced ripple formation — ●HENRI HANSEN, ALEX REDINGER, GEOIGIANA STOIAN, SEBASTIAN MESSLINGER, and THOMAS MICHELY — I.Physikalisches Institut. RWTH Aachen. 52056 Aachen

Pattern formation by 5 keV Ar⁺ ion bombardement at an angle of 83° with respect to the surface normal was studied in the temperature range from 250 K to 720 K.

The nature and density of defects in the ensuing ripple patterns was quantitatively analysed and correlated with the surface morphological evolution. For fixed fluence of 20 MLE a sudden increase in normalized defect density above 450 K is attributed to the onset of step edge diffusion, which tends to align ripple crests along $\langle 110 \rangle$ -direction, whereas ion beam forces the ripple crests to orient along the $\langle \bar{1}\bar{1}2 \rangle$ -direction. Defects in the pattern are spots of high local roughness and thus contribute significantly to the increase of pattern roughness above 450 K.

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Multicomponent nanowires formed by nano shadow masks based on delamination — ●RAINER ADELUNG, MADY ELBAHRI, SHIVA KUMAR RUDRA, ABHIJIT BISWAS, and RAINER KUNZ — Lehrstuhl für Materialverbunde, Technische Fakultät der Universität Kiel, Kaiserstrasse 2, 24143 Kiel, Germany

Simple ways to realize aligned nanostructures are still of interest, as conventional sub 100nm photolithography is not handy with respect to different materials or everyday lab use. Recently, we could show that directed fracture in thin films can be used to fabricate various nanowire structures [1]. But limits of the approach are for example the fabrication nanowires of two different materials in a distance of a few nanometer. Many deficiency like this can be overcome, by being more destructive and going beyond thin film fracture. Adding delamination at the crack sides produces nanoscale shadow masks that create a workspace, allowing to deposit material for multicomponent nanowires, or removing material to trench nanochannels. Various examples of nanostructures will be shown and their application for e.g. sensors or as templates for biological samples will be discussed.

[1] R. Adellung et al., Nature Materials 3, 375, (2004)

O 19.9 Sa 12:45 TU EB420

STM-based nanolithography of diamond-like carbon films — ●THOMAS MÜHL — IFW Dresden, Helmholtzstr. 20, D-01069 Dresden

The spatially localized emission current of a scanning tunneling microscope tip leads to a local graphitization of diamond-like carbon thin films. Using this technique, lines and dots smaller than 10 nm in size can be written. Time resolved studies of the nanostructure growth under the STM tip will be presented, as well as time resolved graphitization of macroscopic areas of metal-contacted diamond-like carbon films induced by high current densities. Due to the widely different properties of diamond-like and graphite-like carbon, there are a lot of possible applications for such graphite nanostructures on diamond-like films. In addition, metal nanowires and nanodots can be produced by shadow (shallow angle) deposition on these carbon nanostructures.