

O 17 Adsorption II

Time: Tuesday 11:15–13:00

Room: TRE Phys

O 17.1 Tue 11:15 TRE Phys

FORMATION OF ULTRATHIN CdS-FILMS ON Cu(111) - AN IN-SITU STM and EX-SITU SXPS STUDY — ●SASCHA HÜMANN¹, PETER BROEKMANN¹, RALF HUNGER², THOMAS MAYER², WOLFRAM JAEGERMANN², and KLAUS WANDEL¹ — ¹Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn — ²Institut für Materialwissenschaft, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt

Electrochemical Atomic Layer Epitaxy is a useful method to grow thin layers of semiconductor compounds at solid/liquid interfaces. In this contribution we present combined ECSTM and synchrotron x-ray photoelectron spectroscopy (SXPS) data dealing with the epitaxial growth of ultrathin CdS-films on a Cu(111) electrode surface. We observed that the atomic structure and the morphology of the resulting CdS film strongly depend on the first layer adsorbed on the copper substrate. The first preparation route of the CdS-films started with a ($\sqrt{7}\times\sqrt{7}$)R19.1° sulfide adlayer on the Cu(111) surface. This root 7 phase could be maintained upon emersion and successfully transferred into the UHV. We observed corresponding LEED images and SXPS data supporting the results of the ECSTM studies. Cd deposition on the root 7 sulfide phase at a potential of -375 mV vs. RHE results in the formation of a CdS-phase revealing a complex dislocation network. After transfer to UHV the composition and chemical nature of the film constituents was analysed. A different CdS phase was obtained when sulfide anions were adsorbed on the Cd precovered copper surface. The corresponding LEED pattern shows a ($\sqrt{3}\times\sqrt{3}$)R30 unit cell.

O 17.2 Tue 11:30 TRE Phys

Correlation of Structure and Femtosecond Electron Dynamics during Crystallization of Amorphous D₂O/Cu(111) — ●JULIA STÄHLER¹, MICHAEL MEHLHORN², UWE BOVENSIEPEN¹, KARINA MORGENSTERN², and MARTIN WOLF¹ — ¹Freie Universität Berlin, Fachbereich Physik, Arnimalle 14, 14195 Berlin, Germany — ²Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Germany

The structure, i.e. molecular arrangement, of an adsorbate layer strongly influences the electron transfer dynamics across the interface since it determines bond strengths and periodicity of the lattice and therefore localized and delocalized states in the adlayer. Using two techniques, low-temperature scanning tunneling microscopy (STM) and time-resolved two-photon photoelectron (2PPE) spectroscopy, we investigate the correlation of the structure and electron dynamics in ultrathin D₂O layers on Cu(111). We find that crystallization of initially porous amorphous ice clusters, which are adsorbed at $T < 90$ K, occurs via three metastable phases. The latter are prepared by annealing to 118 K, 131 K, and 145 K. The stable, crystallized phase is reached by heating to 149 K. These different stages of crystallization are characterized by clear changes in the time-dependent photoelectron spectra. We observe that localization probability and lifetime of the solvated electrons, which are highly sensitive to changes in their local molecular surrounding, strongly depend on the ice structure. Additionally the dependence of image potential states on the ordering in the D₂O layer will be discussed.

O 17.3 Tue 11:45 TRE Phys

Energy resolved quadrupole alignment of H₂ desorbing from Cu(100) — ●CARSTEN THEWES, MARCO RUTKOWSKI, and HELMUT ZACHARIAS — Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster

Measurements of the energy dependent quadrupole alignment for associative desorption of H₂ from Cu(100) were performed. The analysis includes different rotational states in the vibrational ground state $v''=0$ and the first vibrationally excited state $v''=1$. State selective detection of the desorbing molecules is realised by the (VUV+UV)-REMPI techniques. For the excitation step in the $B^1\Sigma_g^+ \leftarrow X^1\Sigma_u^+$ Lyman bands of H₂ photon energies around 110 nm are used. In $v''=0$ the angular momenta $J=1,2,3,4,5$ and 8 while in $v''=1$ measurements for $J''=2,3,4$ could be detected. The acquired energy dependent alignment factor $A_0^{(2)}$ shows a preferentially positive value between 0,2 and 0,4, thus helicopter motion of the desorbing molecules is observed. $A_0^{(2)}$ increases at low kinetic energies close to the respective translational barrier of the two states, i.e. around 300 meV and 200 meV for $v''=0$ and 1, respectively. For

higher energies (1100 meV for $v''=0$, 800 meV for $v''=1$) a decrease of the quadrupole alignment is observed, as expected. Based on theoretical calculations of the quadrupole alignment [1] possible reaction mechanisms will be discussed.

[1] M.F. Somers, D.A. McCormack, G.J. Kroes, R.A. Olsen, E.J. Baerends and R.C. Mowrey; J. Chem. Phys., 117, 6673 (2002)

O 17.4 Tue 12:00 TRE Phys

Adsorption and C 1s NEXAFS Spectra of Three Phenylpropenes on Cu(111) — ●C. KOLCZEWSKI¹, F. J. WILLIAMS², R. L. CROPLEY², R. M. LAMBERT², and KLAUS HERMANN¹ — ¹Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — ²Department of Chemistry, University of Cambridge, Cambridge CB2 1 EW, UK

In this study we present equilibrium geometries of trans-methylstyrene, α -methylstyrene and allylbenzene adsorbed on Cu(111) obtained from density functional theory (DFT) calculations using Cu₇₃-C₉H₁₀ clusters. All molecules are found to adsorb with their phenyl ring lying flat on the surface. However, the position of the side chain varies: allylbenzene adsorbs with its propenyl chain pointing away from the surface whereas for trans-methylstyrene and α -methylstyrene the side chains are closer to the surface but differ in their relative arrangement of C=C bonds and allylic hydrogens. These results can explain the different epoxidation rates measured for the three molecules by simple geometric arguments. The calculated geometries are also used to evaluate theoretical angle resolved C 1s NEXAFS spectra which can be compared with experimental spectra and yield excellent agreement. This confirms the adsorption geometries obtained in the present study and underlines the geometric interpretation of the epoxidation behavior of the phenylpropenes.

O 17.5 Tue 12:15 TRE Phys

LT-STM study of electronic and vibronic properties of single C₆₀ on Cu(111) and Ag(100). — ●ANNA STRÓZECKA, JOSEF MYSLIVEČEK, and BERT VOIGTLÄNDER — Institut für Schichten und Grenzflächen (ISG3), Forschungszentrum Jülich, D-52425 Jülich

A low temperature scanning tunneling microscope (LT-STM), due to its high stability, allows addressing single molecules on the surfaces. Density of States (DOS) spectrum of C₆₀ on Cu(111), measured by STS (Scanning Tunneling Spectroscopy) technique, shows features corresponding to molecular orbitals of a free molecule. The shifting and splitting of the peaks indicate charge transfer from the substrate to the fullerene cage. Peaks in the IETS vibrational spectrum (Inelastic Electron Tunneling Spectroscopy) can be assigned to the vibrational modes of C₆₀. Two different intramolecular modes are observed: $H_g(\omega_2)$ and $H_g(\omega_5)$.

The lateral manipulation was used to precisely control the position of C₆₀ on Ag(100). The plot of the tip height during the manipulation shows that the buckyballs are pulled along the surface.

O 17.6 Tue 12:30 TRE Phys

Vibrations of ethylene on smooth and roughened single crystal copper surfaces — ●MARTIN BINDER, OLAF SKIBBE, and AN-NEMARIE PUCCI — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

The adsorption of ethylene on cold evaporated and annealed copper surfaces and on copper single crystal surfaces has been investigated with Raman spectroscopy and infrared reflection absorption spectroscopy in the past [1]. In order to clarify some remaining questions concerning the assignment of the spectral features to the adsorption sites, we performed high resolution electron energy loss spectroscopy (HREELS) on smooth and slightly roughened single crystal surfaces. Roughening was achieved by utilising ion bombardment without adjacent annealing and evaporating small amounts of copper at low temperatures, respectively. [1] C. Siemes, A. Bruckbauer, A. Goussev, A. Otto, M. Sinther, and A. Pucci. J. Raman Spectrosc. 32 (2001), 231-239 and references therein

O 17.7 Tue 12:45 TRE Phys

Velocity distributions of NO desorbed from C₆₀/Cu(111) by UV laser excitation — •DANIEL GRIMMER, TIM HOGER, and HELMUT ZACHARIAS — Westfälische-Wilhelms Universität, Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster

NO laser desorption experiments have been performed using C₆₀ grown on a poly-Cu cristal. A bimodal distribution of the kinetic energy results in a fast and a slow channel. The fast channel peaks at a velocity of $v=1000$ m/s for low rotational states and increases to 1300 m/s for high rotational states. The slow channel's velocity can be fitted by a Maxwellian flux distribution of $T_{kin}=110$ K showing deviations at slow velocities (Surf. Sci., submitted).

For C₆₀ epitaxially grown on Cu(111) similar results with respect to the kinetic energies and rotational population are obtained. A slightly higher vibrational population is detected.

In these experiments the velocity was inferred from the arrival time in a pump-probe arrangement. The transformation of the delay into a velocity distribution then yields very slow molecules, too slow to be explained by thermal desorption since the kinetic temperature is clearly much below the surface temperature. Diffusion processes or long-lived excited states could cause such a delayed desorption.

Here we present new velocity distributions of NO desorbed from C₆₀/Cu(111) directly measured by a field-free flight time tube.

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