O 55 Epitaxie und Oberflächenreaktionen

Zeit: Mittwoch 10:45–13:00 Raum: TU EB107

O 55.1 Mi 10:45 TU EB107

Surface diffusion and nucleation on Si(111) and Ge(111) 7x7 reconstructed surfaces — •Vasily Cherepanov, Sergey Filimonov, and Bert Voigtländer — Institut für Schichten und Grenzflächen ISG 3, Forschungszentrum Jülich, 52425 Jülich, Germany

Submonolayer deposition on the 7x7 reconstructed Si and Ge surfaces results in formation of two types of objects: the usual 2D islands and small metastable clusters occupying the half unit cells of the surface reconstruction. Using a coarse grain approach we propose a theoretical model with a unified treatment of the coupled system of small clusters and 2D islands. It follows from the model that the densities of 2D islands and small clusters are determined by competition for adatoms. The main energetic parameters determining the measured densities are the diffusion barrier for a single adatom, the energy barrier to reorder the stacking fault unit of the surface reconstruction, and the binding energy of adatoms to the stable small clusters. Simultaneous measurements of the density of 2D islands and the density of small clusters with scanning tunneling microscopy are used to estimate the relevant energetic barriers and to reveal on a quantitative level the influence of the compressive strain, film/substrate material, and surface reconstruction on the island formation and growth.

O 55.2 Mi 11:00 TU EB107

A kmc study of the steering effect in Cu(001) homoepitaxy — •Frits Rabbering, Herbert Wormeester , and Bene Poelsema — MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

One of the key assumptions in the description of growth is the homogeneous distribution of the incoming particle flux. The analysis of high resolution LEED measurements after the deposition of 40 ML of Cu on Cu(001) at various polar deposition angles led to the conclusion that attractive forces between the surface and the incoming particle have a dramatic effect on the trajectory of the incoming particle, called steering [1]. The result of the steering effect is that incoming particles are attracted towards protruding structures. This leads to an increased roughening with pronounced changes in morphology for glancing incidence deposition. The steering effect introduces two additional parameters in the growth process: the polar angle of incidence and the velocity of the incident particles. We developed a Kinetic Monte Carlo program that describes well the growth at normal incidence (only small influence of steering). The first results on the influence of both polar incidence angle and the velocity of the incoming particles on the growth morphology in the temperature range of 180 to 250K will be presented. [1] S. van Dijken, L.C. Jorritsma and B. Poelsema, Phys. Rev. Lett. 82 4038 (1999)

O 55.3 Mi 11:15 TU EB107

A Theoretical study of Nanoporous Carbon for Styrene Catalysis — •Johan M. Carlsson[1], Suljo Linic[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109-2136, USA

Dehydrogenation of Ethylbenzene(EB) to produce Styrene is one of the most important processes in chemical industry. Iron-oxide is widely used as catalyst, but it has recently been proposed that Nanoporous carbon (NPC) deposited on the surface is the actual active material for this reaction. We have therefore studied how motives present in NPC, can change an inert graphene sheet into a chemically active NPC. Our Density Functional Theory (DFT) calculations shows that undercoordinated C-atoms surrounding a vacancy tend to rebind next-nearest neighbours (NNN) forming a larger pore like, structure in the graphene sheet. The strain in the lattice prevent the NNN to form proper sp^2-bonds, such that the defects lead to local curvature and lattice contraction. The cohesive energy of such a defective graphene sheet is comparable to perfect nanotubes in spite of the large E_{form} for the individual defects. This suggests that NPC may concist of graphitic sheets with a significant amount of defects frozen in during growth. The presence of these defects may leave dangling bonds and perturbs the π-band such that a defect state appears close to E_F. Subsequent calculations for oxidation of NPC has confirmed that the vacancies has an increased activity towards adsorption of O_2. These oxidized vacancies furthermore appears promissing as an active sites for oxidative dehydrogenation of EB.

O 55.4 Mi 11:30 TU EB107

Static and Dynamic Self-Organization of Dendron Monolayers on Graphite Monitored with Scanning Tunneling Microscopy — •B. A. Hermann[1], L. Merz[2], L. J. Scherer[3], C. E. Housecroft[3], and E. C. Constable[3] — [1]Dept. of Physics / CeNS, LMU Munich and WMI,Walther-Meissner-Str. 8, 85748 Garching, Germany — [2]on leave from: Inst. of Physics, Uni. Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Dept. of Chemistry, Uni. Basel, Spitalstrasse 51, 4056 Basel, Switzerland

The direct imaging of chemical species at molecular and submolecular levels allows to probe self-organized structures using scanning tunneling microscopy (STM). The evaporation of solutions of bipyridine-dendrons and dendron wedges on graphite give highly ordered monolayers.

The near atomic resolution of the 1st and 2nd generation bipyridine dendron permits us to assign conformers, which spontaneously and rapidly form molecular domains under ambient conditions. Within a molecular domain, only one conformer is present and domains of different conformers are observed side by side. No preference for one conformer was observed.

The long-chain alkyl-decorated Fréchet-type dendron wedges initially form a pattern based on trimeric units, organized into hexagonal host structures with a pseudo-unit cell of seven molecules, one of which remains highly mobile. Over time, it changes into a dimeric pattern. The chirality arising from the adsorption of the dendrons onto the surface is discussed.

O 55.5 Mi 11:45 TU EB107

Water Formation from H_2 ad O_2 on Pt(111) — •Timo Jacob[1,2] and William A. Goddard III.[1] — [1]MSC, Caltech, Pasadena, USA — [2]Fritz-Haber-Institut der MPG, Berlin, Germany

Using density functional theory (DFT) with the B3LYP gradient-corrected exchange-correlation functional, the reaction of $H_2 + {}^1\!/_2 O_2 \longrightarrow H_2O$ was studied on Pt(111), which was represented by a 35 atom cluster. In order to study possible reaction pathways, first binding structures and energetics of each possible intermediate were calculated separately (O, H, O_2, H_2, OH, OOH, H_2O) and afterwards combined with the corresponding dissociation barriers.

Between the two dominant reaction pathways the rate-determining step of the O_2-Dissociation is $O_{ad} + H_{ad} \longrightarrow OH_{ad}$ with a barrier of 31.66 kcal/mol. Along the OOH-Formation pathway $OOH_{ad} \longrightarrow OH_{ad} + O_{ad}$ dissociation has the highest barrier with 17.13 kcal/mol. Although the OOH-Formation is preferred, the oxygen atom, which remains after this reaction without further use, would lead to surface termination. Thus, it also has to use the other reaction channel, or recombine to O_2, which then can be used within the OOH-Formation process.

O 55.6 Mi 12:00 TU EB107

Das Wachstum von Titandioxid auf einer Re(10-10) und einer Ru(0001) Oberfläche — •Dirk Rosenthal[1], Wilhelmine Kudernatsch[1], Klaus Christmann[1], Harry Hoster[2], Hubert Rauscher[2] und R. J. Behm[2] — [1]FU Berlin, Institut für Chemie, Bereich Physikalische und Theoretische Chemie, 14195 Berlin — [2]Abt. Oberflächenchemie und Katalyse, Universität Ulm, 89069, Ulm

Im Rahmen einer Studie zur CO-Oxidation auf goldgeträgertem Titandioxid wurden Titandioxidfilme durch Koadsorption von Titan und Sauerstoff auf einer „glatten“ Ru(0001) und einer grabenförmigen Re(10-10) Oberfläche dargestellt. Morphologie und Wachstum dieser Filme wurden mit LEED, XPS, STM und LEIS untersucht. Auf beiden Substraten wächst Titandioxid in einem Stranski-Krastanov-Modus auf, wobei die benetzende Schicht eine andere Struktur besitzt als die Inseln. Während sich auf dem Ru-Substrat die thermodynamisch günstigste Oberfläche (Rutil(110)) ausbildet, führt die Grabenstruktur des Rheniums zu einer Titandioxidstruktur mit einer Gleitspiegelebene. Sowohl die Rutil(011) als auch die Brookit(001) Oberfläche besitzen diese Symmetrieeigenschaft. Die Einheitsmasche der (2x1) rekonstruierten Rutil(011) Oberfläche ist praktisch gleich groß wie die von Brookit(001). Die Nichtunterscheidbarkeit mit „normalen“ Methoden der Surface Science als auch die Wahrscheinlichkeit des Brookit-Wachstums werden genauso wie der Substrateinfluss diskutiert.

O 55.7 Mi 12:15 TU EB107

Etch figure analysis by scanning force microscopy — •Christian Motzer and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

The method of etching crystals was established to determine crystalographic information like orientation of unknown crystals and later to detect structural defects. Etching analysis strongly assisted the semiconductor industry to produce crystals being free from dislocations and other defects. Analysing etching figures is usually done with optical microscopy hence strongly limited in resolution. For high resolution analysis of etch figures we applied the scanning force microscope. We investigated ex-situ CaF_2(111) cleavage plates which were etched in several acids like sulfuric acid, phosphoric acid, hydrochloric acid and nitric acid. SFM reveals new and profound details of the etched plates which are specific to the surface reaction chemistry which is sensitive to surface and bulk defects. AFM measurements allowed to detect ditrigonal etch pit formation and delayed precipitation formation after etching.

O 55.8 Mi 12:30 TU EB107

Dynamics of Surface Defects observed on CeO_2 (111) by Dynamic Force Microscopy — •S. Gritschneder[1], Y. Namai[2], Y. Iwasawa[2], and M. Reichling[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany — [2]Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

The (111) surface of CeO_2 in various oxidation states is important for catalytic activity and some of its details relating to surface oxygen atoms have already been studied with dynamic scanning force microscopy. The remarkable catalytic properties of ceriumdioxide are strongly connected to the creation, diffusion and healing of oxygen vacancies and, hence, CeO_2 is used as an oxygen storage device in various technical applications like for instance the three-way-catalyst and the solid oxide fuel cell. We demonstrate that dynamic force microscopy is perfectly suitable to investigate nanoscale and atomic size defects on this insulating oxide surface. Our experiments reveal a rich variety of surface defects in form vacancies and protrusions localized at single, well defined lattice sites as well as extended defect formations involving several surface or sub-surface ions. Many of the defects are very stable, but we can show in series of consecutively recorded images that defects can also appear, disappear and change their morphology. Aiming for a chemical identification of the defects, we exposed slightly reduced CeO_{2-x}(111) surfaces to molecular oxygen and observed the changes in the apparent surface structure. Already at very low dosages of less than 10 Langmuir, we observe effects that we interpret as healing of oxygen vacancies.

O 55.9 Mi 12:45 TU EB107

STM studies on the electronic properties of single Au atoms and Au dimers on a thin Al_2O_3 film on NiAl(110) — •Maria Kulawik, Niklas Nilius, Hans-Peter Rust, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Abteilung Chemische Physik, Faradayweg 4-6, 14195 Berlin

The adsorption and diffusion of metal atoms on oxide surfaces play key roles in heterogeneous catalysis, notably for the regeneration of the catalytically active species. Despite the importance of these processes, only little is known on the atomic level, which is mainly due to the high complexity of real catalysts. Therefore, the study of model systems is essential to gain a fundamental understanding of these processes.

Here, we have investigated the electronic structure of single Au atoms on a thin Al_2O_3 film on NiAl(110) by Scanning Tunneling Microscopy and Spectroscopy (STM/STS) at 5 K. STS spectra of Au monomers exhibit single resonances between 2 and 3 eV whereby the energy position depends on the adsorption site. For Au dimers, a split of this peak is observed. Conductance images reveal the spacial distribution of the LDOS.