

tion another approach is chosen and the growth of films deposited on an already rough surface is investigated. Here smoothing phenomena may occur depending on the materials used. As rough substrates thin Ag-films on Si were used, which show distinct island growth and thus exhibit statistic roughness (rms of 0.9 nm). Smoothing is done by deposition of an additional amorphous layer of partially stabilized zirconium oxide (PSZ) with an rms-roughness of 0.1 nm on Si and the results were discussed with respect to the dominating smoothing mechanisms that occur during deposition. Therefore stochastic differential equations were consulted and the scaling behaviour of the roughness evolution was investigated. All samples were deposited by pulsed laser deposition and investigated via atomic force microscopy. Power spectral densities as well as autocorrelation functions were calculated.

O 90.7 Fri 11:45 MA 042

Experimental Observation of Amontonian and Superlubric Sliding in Extended Nanocontacts — •DIRK DIETZEL^{1,2}, TRISTAN MÖNNINGHOFF¹, U. D. SCHWARZ³, CLAUDIA RITTER³, HARALD FUCHS^{1,2}, and ANDRE SCHIRMEISEN¹ — ¹Institute of Physics, University of Münster, Münster, Germany — ²INT, Forschungszentrum

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One of the most fundamental questions in nanotribology is the contact area dependence of frictional forces on the nanometer scale. Unfortunately, conventional friction force microscopy techniques are limited for analyzing this problem due to the unknown and ill-defined tip-sample contact. This limitation can be circumvented by measuring the lateral force signal during the manipulation of nanoscale particles with a well-defined, clean contact to the substrate. In our study, the samples under investigation were metallic islands with diameters between 50-500 nm grown by thermal evaporation of antimony on highly oriented pyrolytic graphite (HOPG). Experiments that included the controlled manipulation of a large number of nanoparticles in ultrahigh vacuum show two distinct frictional states during particle sliding: While some particles show finite friction increasing linearly with interface area, thus reinforcing Amontons's law at the nanoscale, other particles assume a state of frictionless or 'superlubric' sliding. This unexpected duality of friction states can be explained by contamination effects of the interface that alter the frictional properties.

O 91: SYEC: Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations IV (FV: O+HL+DF+TT)

Time: Friday 10:15–12:30

Location: A 151

See SYEC for details about the program.

O 92: SYMS: Modern Developments in Multiphysics Materials Simulations III (FV: O+HL+MM)

Time: Friday 10:15–13:00

Location: A 053

See SYMS for details about the program.

O 93: Surface Chemical Reactions

Time: Friday 10:15–13:00

Location: MA 043

O 93.1 Fri 10:15 MA 043

A two-step mechanism for the oxidation of vacancies in graphene — •JOHAN M. CARLSSON, FELIX HANKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin

Complete oxidation of graphitic carbon materials leads to combustion and the formation of CO₂, but it has been suggested that partial oxidation of vacancies on the basal plane can yield catalytically interesting materials. The characterization of such oxidized graphite in temperature-programmed desorption (TPD) experiments detected a surprising amount of CO and significantly less CO₂ [1]. This work aims to clarify the oxidation mechanisms and surface structures under different experimental conditions. We use density functional calculations with PBE exchange-correlation to obtain the structural and energetic properties of oxidized graphene vacancies. To understand the TPD spectra, reaction barriers and rates for CO and CO₂ desorption are calculated from transition state theory and the nudged elastic band method. An *ab-initio* thermodynamics analysis shows a significant partial pressure-dependence of the oxygen content in vacancies. This indicates a two-step mechanism for the initial oxidation, by which strongly bound CO-releasing C-O-C and C=O groups saturate the vacancies under the ultra-high vacuum conditions of TPD experiments. Atmospheric partial pressures lead to additional oxygen adsorption into extended groups such as C-O-C=O and O=C-O-C=O, which in return can desorb as CO₂. [1] B. Marchon *et al.*, Carbon **26**, 507 (1988).

O 93.2 Fri 10:30 MA 043

Structure and Composition of the TiO₂(110) Surface: From UHV to Realistic Reaction Conditions — •PIOTR KOWALSKI, BERND MEYER, and DOMINIK MARX — Lehrstuhl fuer Theoretische Chemie, Ruhr-Universitaet, D-44780 Bochum, Germany

Using DFT-based *ab-initio* calculations in combination with a thermodynamic formalism we have calculated the relative stability of various

structural models of the nonpolar, mixed-terminated TiO₂(110) surface in contact with a surrounding gas phase at finite temperature and pressure. Adsorption and desorption of hydrogen atoms and water molecules, as well as the formation of O vacancies were considered. Assuming thermodynamic equilibrium between the TiO₂ surface and an oxygen, hydrogen and water containing atmosphere, we constructed a phase diagram of the lowest free energy surface structures.

For a wide range of temperatures and pressures we find that water will be adsorbed at the surface. At full monolayer coverage, a molecular adsorption of water is preferential. The most stable adsorption site for hydrogen atoms is on-top of the bridging O atoms. Surprisingly, we find that in thermodynamic equilibrium the bridging O atoms can not be fully saturated which hydrogen, but only a maximum coverage of about 0.6 monolayer can be reached. The formation energy for O vacancies is found to be rather high so that O defects should only form at extreme oxygen poor conditions.

O 93.3 Fri 10:45 MA 043

Dissociation of oxygen on Ag(100) by electron induced manipulation — •CARSTEN SPRODOWSKI, MICHAEL MEHLHORN, and KARINA MORGENSTERN — Institut für Festkörperphysik, Abteilung Oberflächen, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover, Germany

Low-temperature scanning tunneling microscopy is used to study oxygen dissociation on Ag(100). Deposition of oxygen on Ag(100) at 80K leads to small clusters of 1 to 10 molecules. Inelastic electron tunnelling manipulation is used for the manipulation of these molecules. Thereby the STM tip is set above them, the feedback loop of the STM is switched off and a voltage is applied between tip and sample for exciting the electronic states of the molecules. For small energies (1500meV with 0.3 nA) the cluster reorders, while above a distinct energy threshold the electron induced manipulation leads to a dissociation of the single molecules within the cluster. After manipulation in some cases dissociated pairs at different distances are found. However mostly only one atom of the dissociated molecule is observed.