

O 25: Phase Transitions

Time: Tuesday 11:15–12:45

Location: H41

O 25.1 Tue 11:15 H41

Order-disorder phase transitions: a DFT - (Wang-Landau) MC study — ●MIRA TODOROVA¹, MIKAEL BORG², CATHERINE STAMPFL³, and MATTHIAS SCHEFFLER⁴ — ¹Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf — ²University of Toronto, Toronto, Canada — ³School of Physics, The University of Sydney, Australia — ⁴Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Using a hybrid statistical mechanics method comprising the use of a Lattice-gas Hamiltonian (LGH) determined from density-functional theory and subsequent Monte Carlo (MC) calculations, we obtain a phase diagram for Na-Al surface alloy systems from first-principles and compare it to experimental results [1].

A safe approach towards parametrizing a LGH from the self-consistent evaluation of the electronic structure starts with an analytic form for the long-range pair-interactions. This expression is corrected in the short and medium range using DFT derived data, also including near-sighted many-body terms. An ensuing cross-validation is of utmost importance to ensure that the corrections (to the long-range part) are assessed with an optimum accuracy. The thus extracted LGH is used to perform MC calculations, also using the new Wang-Landau MC algorithm [2], which allows us to reliably determine the transition temperature.

[1] M. Borg, *et al.*, Chem. Phys.Chem. **6**, 1923 (2005).

[2] F. Wang and D.P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).

O 25.2 Tue 11:30 H41

Phase diagram of oxygen adsorbed on Ni(111) and thermodynamic properties from first-principles — ●CESAR LAZO¹ and FRERICH KEIL² — ¹Inst. of Applied Physics, Hamburg University, Jungiusstr. 9a, 20355 Hamburg. — ²Inst. of Chemical Reactions, Hamburg University of Technology, Eissendorfer Str. 38, 21073, Hamburg.

Thermodynamic properties and the surface phase diagram of O/Ni(111) have been calculated from Metropolis and Wang-Landau Monte Carlo simulations based on lateral interactions derived from density functional theory (DFT) calculations. The DFT energies were mapped onto an Ising-like Hamiltonian according to the cluster expansion technique formalism[1]. Both, fcc and hcp adsorption sites were included in the Hamiltonian. Different criteria were used to evaluate competing parameter sets: cross-validation score CV , Malloy's C_p statistics and adjusted R^2 statistics. The parameter space was searched using genetic algorithms in order to find optimum sets. Excellent agreement is found when comparing the shape and stability regions of the theoretical and experimental (from the literature[2]) phase diagrams. Additionally, we were able to elucidate the nature of the $p(2 \times 2)$ phase transition at 1/4 ML oxygen coverage (experimental results in the literature disagree about the nature of this transition). Differences arise when comparing the values of the calculated and experimental transition temperatures owing to imprecision in present-day DFT calculations.

[1] van de Walle *et al.*, J. Phase Equilib. **23**, 348 (2002).

[2] Schwennicke *et al.*, Phys. Rev. B **56**, 224207 (1997).

O 25.3 Tue 11:45 H41

Repulsive interaction between organic molecules upon adsorption: the case of Sn-phthalocyanine/Ag(111) — ●CHRISTOPH STADLER, SÖREN HANSEN, CHRISTIAN KUMPF, and EBERHARD UMBACH — University of Würzburg, Experimental Physics II, 97074 Würzburg, Germany

The properties of organic thin films largely depend on the balance between molecule-molecule and molecule-substrate interactions and often can be tuned by changing the preparation conditions like temperature or coverage. This is also the case for the family of phthalocyanines (Pc), which are frequently studied as adsorbates on various surfaces. Here we present results on SnPc/Ag(111), a non-planar representative of this family. We used high resolution (SPA-)LEED to investigate the phase diagram of the monolayer regime.

At room temperature the adsorbed SnPc molecules show no long-range order in SPA-LEED up to a coverage of about 0.9. Above this coverage, the film forms incommensurate superstructures, the unit cell parameters of which change *continuously* with increasing coverage.

This behavior can be explained by a repulsive intermolecular interaction of the SnPc molecules on the Ag surface. Interestingly, upon cooling below 230 K the film forms a commensurate superstructure between a coverage of 0.6 and 0.9 monolayer.

O 25.4 Tue 12:00 H41

Structural implications of the 1d-2d-transition in Pb wires on Si(557) — ●MARCIN CZUBANOWSKI, SHIMA AKBARI, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik Leibniz Universität Hannover

The adsorption of Pb on Si(557) substrates leads to the formation of anisotropic metallic structures as revealed by conductivity measurements, STM and ARPES. The annealing of at least 1ML Pb to 640K forms atomic chain structures, which show below $T_c=78$ K a metallic conductance along the wires ($\bar{1}10$), whereas in the ($\bar{1}12$) direction an insulating behavior is found. This quasi one-dimensional conductance below T_c is originated by complete Fermi nesting in the direction normal to the structure and split-off valence bands with mesoscopic Fermi-wavelengths along the Pb-chains. These observations are coupled with structural changes that were investigated systematically close to T_c by SPA-LEED experiments described here. The Pb-chains reorganize the structure of Si(557) substrate into [223] facets with $4\frac{2}{3}$ Si unit cells in the $[11\bar{2}]$ direction, as seen by a spot-splitting of 21,3%. This terrace structure undergoes a reversible incommensurate-incommensurate phase transition at T_c , which increases the average interchain distance d and destroys the perfect nesting condition. Simultaneously, the Pb-induced regularly spaced domain wall network, as evident from a 10-fold splitting of the $\sqrt{3}$ structure, disappears. These findings explain qualitatively the observed transport properties, as will be shown.

O 25.5 Tue 12:15 H41

Reversible martensitic phase transition in 4 ML Fe films on Cu(100): A variable temperature STM study — ●ALBERT BIEDERMANN — Institute of Materials Physics, University of Vienna, 1090 Vienna, Austria

In recent years it has been established that 3–4 ML Fe films grown on Cu(100) show a bcc-like structure in terms of crystallography (“nanomartensite”)[1] and electronic structure [2]. This work addresses the question whether there also exists a reversible martensitic phase transition between this bcc-like and the fcc phase. Temperature dependent LEED and SMOKE data by Zharnikov *et al.* [3] suggest a transformation from the ferromagnetic phase to the fcc phase in 4 ML films between 250 and 330 K and a slow reverse transformation after cooling to below 180 K. Indeed, variable temperature STM images obtained in the present experiments show a transition from the bcc-like to the fcc phase between 280 and 330 K in 4 ML films. The reverse transition occurs around 200–250 K on the slow time scale of the VT-STM experiment. This reversible martensitic transition confirms the rather strict correlation between bcc-like structure and ferromagnetic ordering in 4 ML films. The temperature dependent growth of the 2D martensitic “grains” and their characteristic length scales will be discussed.

[1] A. Biedermann, R. Tscheliessnig, M. Schmid, P. Varga, Phys. Rev. Lett. **87** (2001) 086103

[2] D. Spisak, J. Hafner, Phys. Rev. Lett. **88** (2002) 056101

[3] M. Zharnikov, A. Dittschar, W. Kuch, C. M. Schneider, and J. Kirschner, Phys. Rev. Lett. **76** (1996) 4620

O 25.6 Tue 12:30 H41

Temperature Dependent Phase Transitions in 3d-Metal Intercalated Titanium Dichalcogenides — ●EIKE F SCHWIER¹, ANDREAS NUBER¹, SVETLANA TITOVA², ALEXANDER TITOV³, and FRIEDRICH REINERT¹ — ¹Universität Würzburg, Experimentelle Physik II, 97094 Würzburg, Germany — ²Institute of Metallurgy, Urals Division of RAS, Russia — ³Institute of Metal Physics, Urals Division of RAS, Russia

To this day, it is not fully understood why certain titanium dichalcogenides show the presence of superstructures and others do not. By systematically intercalating these layered solids with electrons from 3d-metal atoms, we want to gain a deeper understanding of the electronic and structural processes within these compounds, that lead to the formation of superstructures and their suppression.

Previous conductance measurements suggest a second order phase

transition at 420 K for Ag_xTiTe_2 ($x = 0.65 - 0.74$) and at 120 K for $\text{Mn}_{0.145}\text{TiSe}_2$. By angle-resolved UPS (He I and He II) and XPS (Al K_α) we investigated the influence of the phase transition to the electronic structure along the high-symmetry directions $M-\Gamma-M$ and

$\Gamma-K$ of the two materials and relate it to the band structure calculations, the conductance behavior of electronic structure and structural changes.