

O 18: Metallic Nanowires on Semiconductor Surfaces

Time: Monday 17:00–19:30

Location: Poster A

O 18.1 Mon 17:00 Poster A

Stepped Silicon Surfaces: Exploring the Formation of Spin Chains — JULIAN AULBACH¹, •TIM WAGNER¹, STEVEN C. ERWIN², RALPH CLAESSEN¹, and JOERG SCHAEFER¹ — ¹Physikalisches Institut und Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Germany — ²Naval Research Laboratory, Washington DC, USA

Adsorption of a submonolayer of gold on various stepped Si(hhk) substrates yield the formation of atomic wire arrays with rather perfect structural order. As a specific representative, stabilization of the Si(553) surface by Au adsorption results in two different atomically defined chain types, one made of Au atoms and one of Si. The latter, situated at the step edges, forms a honeycomb nanoribbon which is subject to antiferromagnetic spin ordering [1, 2]. However, the extent to which the magnetic pattern can be modified, or suppressed, has remained unexplored. Here our approach is to exploit the tunability offered by the Si(hhk)-Au family, which exhibits not only varied terrace widths but also different bonding networks. Based on scanning tunneling microscopy and density-functional theory we reveal why magnetic patterns form on particular Si(hhk) surfaces but not on others, and propose broad strategies for using surface chemistry to control the formation or suppression of spin chains more generally.

[1] J. Aulbach et al., Phys. Rev. Lett. 111, 137203 (2013).

[2] S. C. Erwin and F. J. Himpsel, Nat. Commun. 1, 58 (2010).

O 18.2 Mon 17:00 Poster A

Observation of correlated spin-orbit order in a strongly anisotropic quantum wire system — •MONIKA JÄGER, CHRISTIAN BRAND, HERBERT PFNÜR, and CHRISTOPH TEGENKAMP — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Vicinal Si(557) surfaces covered by 1.31 ML Pb reveal a 1D transport behavior below 78 K [1]. The delicate interplay between the superlattice structure, band filling, and extremely large spin-orbit interaction results in a highly correlated entangled spin- and charge-state. Recent spin resolved ARPES measurements have shown that the insulating behavior across the direction of the wires is associated with the formation of a spin-orbit density wave [2, 3].

In order to correlate these findings with the morphology the atomic structure was investigated by means of STM. Adsorption of Pb at 600 K gives rise to a refaceting of the Si surface into a local (223) orientation with an average spacing of 1.58 nm. High resolution STM images have clearly identified $\sqrt{3} \times \sqrt{3}$ reconstructions on the $4\frac{2}{3} \times 0.332$ nm wide (111) terraces. The 0.665 nm periodicity along the terraces is superimposed by an additional intensity modulation which is compatible with a 10-fold periodicity deduced from the spot-splitting seen in former high resolution LEED measurements.

[1] C. Tegenkamp et.al. PRL **95**, 176804 (2005).

[2] C. Brand et.al. Nat. Comm. **6**, 8118 (2015).

[3] C. Tegenkamp et.al. PRL **109**, 266401 (2012).

O 18.3 Mon 17:00 Poster A

Structural and electronic instabilities in Si(hhk)-Au — •MARVIN DETERT, TIMO LICHTENSTEIN, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik, Leibniz Universität Hannover

For future plasmonic devices understanding at low dimensional collective excitations is indispensable. For quasi one dimensional (1d) structures, Au induced wires on regularly stepped Si(hhk) offer the perfect playground. Therefore, Si(553) and Si(775) were prepared at coverages where both surfaces host a double atomic gold chain per terrace. All measurements were performed at a base pressure of 5×10^{-11} mbar by an electron energy loss spectrometer combined with a setup of spot profil analysis in low energy electron diffraction providing both high momentum and energy resolution.

As long time measurements showed a time dependent shift of the plasmon dispersion for Si(hhk)-Au at various Au coverages, the plasmonic excitations in Si(775)-Au and Si(553)-Au, particularly the dispersion relation and its time dependence, were investigated. Primarily we took special care to eliminate water and hydrogen from the background gas. We found that the plasmon dispersion remains unchanged over time for a coverage of 0.48 ML for Si(553)-Au and a coverage of

0.32 ML for Si(775)-Au. Therefore, at these coverages all dangling bonds seem to be saturated. At other coverages, thermal desorption spectroscopy shows mainly an H₂ peak at 580 °C. Therefore, we conclude that atomic hydrogen generated by the electron beam leads to a modification of structural and electronic properties.

O 18.4 Mon 17:00 Poster A

Local defects in quasi-1D Si(553)-Au — •ZAMIN MAMIYEV, TIMO LICHTENSTEIN, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Self-assembled quasi-1D metallic structures formed on vicinal Si surfaces are highly attractive due to their individual electronic states that are confined to a single spatial dimension. In this respect, metallic nanowires induced by Au atoms at the regularly stepped Si(553) surface exhibit a variety of interesting electronic properties which are determined by the atomic structure. In order to obtain a quantitative description of the chemically adsorbed residual gas (CO, H₂O, H₂) effect to plasmon loss, time dependent electron energy loss spectra were measured along the momentum transfer parallel (q_{\parallel}) and perpendicular (q_{\perp}) to wires. Plasmon loss energy shows a linear decay of the adsorption probability as a function of active site concentration, and an exponential saturation of the additional coverage with time.

On the Si(553)-Au surface Au atoms are arranged in dimerized double chains per terrace and show a strong tendency to suffer structural transitions. Since the whole terrace is chemically active on the Si(553)-Au surface, it is conceivable that an adsorption of the additional atoms takes place on these chains. Due to strong chemical bonds, atomic hydrogen locally converts the Au chains into an insulator. Therefore, the atomic hydrogen adsorbed on the surface is limiting the propagation of collective modes.

O 18.5 Mon 17:00 Poster A

Au/Si(553) and Au/Si(111) surface phonons and Raman scattering efficiencies calculated from first principles — •SERGEJ NEUFELD, SIMONE SANNA, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn

Metallic nanowires on semiconducting substrates have been attracting considerable interest in the last decades. Self organizing gold chains at vicinal surfaces such as the Si(553) and Si(111) are of particular interest, as the use of stepped templates allows to vary the geometric parameters and, thus, tune the inter-chain coupling. While microscopic structural models of Au nanowires on various Si surfaces are available in the literature, little is known about their vibrational properties in terms of surface localized phonon mode frequencies, eigenmodes and Raman scattering efficiencies. In this work, the phonon mode characteristics of the Au/Si(553) and Au/Si(111) surfaces are calculated from first-principles. Several surface localized phonon modes are found, whose phonon frequencies can be directly compared with the spectra obtained by Raman measurements. Additionally, the differential Raman cross section of the Au/Si(111) surface is calculated via linear response routines. A qualitative agreement between theoretical and experimental spectra could be observed.

O 18.6 Mon 17:00 Poster A

Au nanowires at Si(775): Structure, electronic bands and magnetic ordering calculated from first principles — •CHRISTIAN BRAUN, SIMONE SANNA, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

In recent years, one-dimensional systems have increasingly come into focus due to their interesting electronic properties including, inter alia, Peierls instabilities and Luttinger liquid behavior. Promising realizations of quasi-one-dimensional systems are, among others, self-assembled gold nanowires on vicinal Si(111) surfaces.

However, the exact structure of many gold deposited vicinal Si(111) surfaces are still unclear. In this work, various structures of gold chains on the Si(775) surface have been investigated by first-principles and, depending on the gold coverage, different models for this particular surface are proposed. These are supported by STM simulations and calculations of the band structure. Interestingly, we find the energetically most favored models to show a magnetic ordering, similar to the case of Au/Si(553) surface [1].

[1] SC Erwin, FJ Himpsel, Nature Commun. 1, 1 (2010).

O 18.7 Mon 17:00 Poster A

SPA-LEED investigations of quasi one dimensional Dysprosium silicide structures on Si(001) — ●JASCHA BAHLMANN, FREDERIC TIMMER, and JOACHIM WOLLSCHLÄGER — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

The investigation of rare earth metal induced nanowires on silicon is of particular interest due to their quasi one dimensional structure and the consequential electronic properties. Dy was deposited on flash-annealed Si(001) samples by means of physical vapor deposition (PVD) and examined by spot profile analysis low energy electron diffraction (SPA-LEED) as a function of the Dy coverage and the sample temperature.

(2×4) - and (2×7) -reconstructions are observed at lower coverages. The formation of these structures appears to be temperature-dependent. A bundling of the nanowires can be observed at sample temperatures of 500° C and higher coverages. In addition mean domain sizes were determined in order to derive the optimal growth parameters for the nanowires.

O 18.8 Mon 17:00 Poster A

Structural and electronic properties of rare-earth silicide thin films at Si(111) — ●CHRISTOF DUES, WOLF GERO SCHMIDT, and SIMONE SANNA — Lehrstuhl für Theoretische Physik, Universität Paderborn, D-33095 Paderborn

Rare-earth (RE) silicides thin films on silicon surfaces are currently of high interest. They grow nearly defect-free because of the small lattice mismatch, and exhibit very low Schottky-barriers on n-type silicon. They even give rise to the self-organized formation of RE silicide nanowires on the Si(001) and vicinal surfaces.

Depending on the amount of deposited RE atoms, a plethora of reconstructions are observed for the RE silicide. While one monolayer leads to the formation of a 1×1 -reconstruction, several monolayer thick silicides crystallize in a $\sqrt{3} \times \sqrt{3}$ R30° superstructure. Submonolayer RE deposition leads to different periodicities.

In this work we investigate the formation of RE silicides thin films on Si(111) within the density functional theory. The energetically favored adsorption site for RE adatoms is determined calculating the potential energy surface. As prototypical RE, Dysprosium is used. Additional calculations are performed for silicides formed by different RE elements. We calculate structural properties, electronic band structures and compare measured and simulated STM images. We consider different terminations for the 5×2 reconstruction occurring in the submonolayer regime and investigate their stability by means of *ab initio* thermodynamics. The same method is employed to predict the stable silicide structure as a function of the deposited RE atoms.

O 18.9 Mon 17:00 Poster A

Raman spectroscopy of quasi-1D nanowires on the Si(553)-Au surface — ●JULIAN PLAICKNER¹, SANDHYA CHANDOLA¹, EUGEN SPEISER¹, NORBERT ESSER¹, BENEDIKT HALBIG², JEAN GUERTS², JULIAN AULBACH³, JÖRG SCHÄFER³, SERGEJ NEUFELD⁴, and Si-

MONE SANNA⁴ — ¹Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Berlin — ²Universität Würzburg, Experimentelle Physik III, Würzburg — ³Universität Würzburg, Experimentelle Physik IV, Würzburg — ⁴Fakultät für Naturwissenschaften, Department Physik, Universität Paderborn

Vicinal Si(111) substrates offer an additional control parameter (terrace width) for growth of atomic gold chains on Si(111) terraces. Moreover, a new one-dimensional so-called Si honeycomb-like structure is generated, the latter exhibiting spin polarization effects at low temperature, according to calculations [1], accompanied by small structural changes at the step edges. Optical methods such as Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy have been shown to be sensitive tools to verify surface structure of such nanostructures. Here we concentrate on a study of the surface phonon modes of the Si(553)-Au-(5x2) surface by Surface Raman Spectroscopy.

Raman spectra Si(553)-Au-(5x2) surface show clear signatures of Au- and Si related surface vibrations, while RAS shows signatures of electronic surface transitions [2]. Additionally, the measurement of Raman spectra for different polarization configurations allows investigating the symmetry of the phonon modes. The comparison of Raman spectra taken at room temperature and low temperatures shows clear differences that can be related to specific structural elements of the surface. This suggests that a structural transition occurred between the two temperatures.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. 1, 58 (2010)

[2] C. Hogan et al. PRL 111, 8, 087401 (2013)

O 18.10 Mon 17:00 Poster A

Optical properties and electronic doping of quasi-1D gold nanowires on vicinal Si surfaces — ●SANDHYA CHANDOLA¹, EUGEN SPEISER¹, JULIAN PLAICKNER¹, CONOR HOGAN², JULIAN AULBACH³, JÖRG SCHÄFER³, and NORBERT ESSER¹ — ¹Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — ²Institute for Structure of Matter, National Research Council (CNR-ISM) Via Fosso del Cavaliere, 00133 Rome, Italy — ³Universität Würzburg, Experimentelle Physik IV, Würzburg

The atomic structures of sub-monolayers of gold on vicinal Si surfaces are currently under intense discussion. Such structures can be investigated in microscopic detail by optical techniques such as Reflection Anisotropy Spectroscopy (RAS), which is extremely sensitive to the 1D nature of these systems. It will be shown that the local electronic properties of these surfaces can be tuned by controlled doping of hydrogen. The optical response of the clean Si(553), Si(553)-Au and hydrogenated Si(553)-Au surfaces are measured with RAS and compared with density functional theory (DFT) simulations. By analysing the optical response of the freshly prepared and hydrogenated Si(553)-Au surfaces, the spectral features can be directly attributed to specific atomic-scale structural elements on the surface. Hydrogen adsorption is shown to attenuate the response at spectral regions associated with the honeycomb chains at the Si step edges. The doping process is reversible and can be used as a controllable parameter to tune the electronic properties of this system.