DS 45: Poster IV: One-Dimensional Metals: Reality or Fiction

Time: Thursday 16:00–19:00 Location: P1

DS 45.1 Thu 16:00 P1

Structural investigations of Au quantum wires on Ge(100) — •Heiko Teiken, Timo Lichtenstein, Christoph Tegenkamp, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, AbteilungATMOS, 30167 Hannover

Ge(100) is known as a substrate for self-organized growth of one dimensional quantum wires by adsorption of Au. As shown recently (C. Blumenstein et.al. Nature 7, 776) the signatures of a Luttinger liquid behavior depends crucially on the quality of the ensemble and, consequently, on the quality of the Ge(100) sample prior to adsorption. Furthermore, there is a debate regarding details of the atomic structure of the atomic wires induced upon Au adsorption. In this study we have measured systematically roughness parameters on variously prepared surfaces by means of spot profile analysis of low energy electron diffraction patterns (SPA-LEED). From G(S)- and H(S)-analyses Gemonoatomic step heights of 1.42$\AA$ with average terrace lengths around 20 nm are found. Ex-situ chemically treated Ge-samples followed by in-situ thermal annealing reveal slightly lower rms-values (1.3 Å) as samples which have undergone multiple in-situ sputter/annealing cycles. The G(S)-curves reveal additional structurs after growth of the Au-wires corresponding to step heights of 1.8 Å which we suggest to be due to interference between gold covered islands and clean terraces. The overall roughness of the Ge-template does not increase due to growth of the Au-induced wires. Details of the G(S)-curves will be discussed in terms of different structural models (Au-dimer chains vs. Au-induced Ge-facet structures) currently proposed in literature.

DS 45.2 Thu 16:00 P1

Structural and electronic properties of Si(111)-(5×2)-Au surface from first-principles calculations — •Kaori Seino and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany

Self-assembled atomic wires fabricated on semiconductor surfaces are promising candidates for future nanoelectronics. The Si(111)-(5×2)-Au surface is one of the examples where atomic nanowires appear. For a long time it has been the subject of experimental and theoretical studies. The experimental determination of the Au coverage has been recently revised to be 0.6 ML instead of 0.4 ML. Correspondingly, a structural model was proposed from first-principles calculations [1]. However, recently an alternative model is proposed from structural studies [2]. Still the surface reconstruction of the Si(111)-(5×2)-Au surface is under debate.

Here we present *ab-initio* calculations of structural and electronic properties of Si(111)-(5×2)-Au. To assess the accuracy of our first-principles total energy methods, we also used different exchange correlation functionals including the Perdew-Becke-Ernzerhof functional for solids and surfaces (PBEsol) and the van der Waals density functional (vdW-DF). We clearly favor the model proposed by Erwin *et al.* [1] versus that proposed by Abukawa and Nishigaya [2].

[1] S. C. Erwin *et al.*, Phys. Rev. B **80**, 155409 (2009).
[2] T. Abukawa und Y. Nishigaya, Phys. Rev. Lett. **110**, 036102 (2013).

DS 45.3 Thu 16:00 P1

Rare Earth Silicides from Density Functional Theory — •Kris Holtgrewe, Simone Sanna, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany

Rare earth silicide nanowires are of high interest both because of their fundamental physics properties and for applications such as nanoscale interconnects, optical waveguides and quantum devices. However, the exact knowledge of their atomic structure is still incomplete. The detailed knowledge of the bulk phase of the rare earth silicides is a prerequisite for a fundamental understanding of the ground and excited state properties of the nanowires. As a first step towards the nanowire modeling, we have investigated the hexagonal and tetragonal phases of several rare earth disilicides, including $ErSi_2$, $DySi_2$ and $HoSi_2$ from *first-principles*. The $4f$ electrons of the rare earth are treated both as valence states, explicitly taking into account the on-site Coulomb interactions, or as frozen state in the atomic core. Structural and electronic properties of the investigated systems are discussed. While all the silicides are characterized by rather similar lattice parameters, these are found to strongly depend on the Si vacancy concentration.

DS 45.4 Thu 16:00 P1

Tb silicide nanowires on planar and vicinal Si(001): growth and characterisation — •Stephan Appelfeller, Stefan Kuls, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Deutschland

Metallic nanowires are interesting not only because of their possible future applications in nanoelectronics but also because of unique one-dimensional phenomena, e.g. the Peierls instability or Luttinger liquid behavior. A model system for metallic nanowires are silicide nanowires on Si(001). Here, the growth of Tb silicide structures by molecular beam epitaxy on planar and vicinal Si(001) surfaces was studied for the first time. Submonolayer amounts of Tb were deposited at room temperature and subsequently annealed at elevated temperatures. A wire-like 2×7 reconstruction and – for coverages surpassing a critical coverage – Tb silicide nanowires were observed and analysed by scanning tunnelling microscopy. The critical coverage reduces for more structured surfaces, e.g. vicinal surfaces. At moderate annealing temperatures, the 2×7 reconstruction, which shows a strongly voltage dependant appearance, remains intact upon nanowire formation. In contrast, the 2×7 reconstruction disappears during nanowire formation at higher temperatures. The structure of the nanowires could be identified as hexagonal $TbSi_2$. They are highly anisotropic with widths of few nanometers and lengths of several hundred nanometers and grow parallel to each other on well ordered vicinal surfaces. This work was supported by the DFG through FOR 1700 project E2.

DS 45.5 Thu 16:00 P1

Pb nanowires on Si(557) — •Frederic Timmer[1], Sebastian Gevers[1], Thomas Weisemöller[1], Christoph Tegenkamp[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover

The restructuring of the Si(557) surface during formation of Pb nanowires has been investigated in-situ by surface x-ray diffraction (SXRD) studies which were performed at the beamline ID03 of ESRF. For this purpose, Pb has been deposited on the bare Si(557) - (3×1) at room temperature until 3D Pb islands were grown on the initial Pb wetting layer. The formation of Pb islands was monitored by the appearance of 3D Pb Bragg peaks.

Thereafter, Pb was carefully desorbed by annealing to 600K. This process was controlled by recording corresponding 3D Pb Bragg peaks directly in-situ by SXRD. Desorption of Pb has been stopped when the Pb islands have vanished and the Pb wetting layer is transformed into a $\left(\sqrt{3}\times\sqrt{3}\right)$ superstructure on the nano-(111) terraces of the Si(557) surfaces. Reciprocal space mappings were recorded in the $[7,7,\bar{10}]$ direction, i.e. perpendicular to the atomic steps, clearly indicating a strong refacetting of the initial (557) orientation. It turns out that the restructured Si(557) surface is indeed stabilized by the $\left(\sqrt{3}\times\sqrt{3}\right)$ Pb overlayer on the Si(111) terraces.

DS 45.6 Thu 16:00 P1

Structural studies on self-assembled atomic gold nanowires of the Si(111)-(5x2)-Au reconstruction by Surface X-Ray Diffraction — •Patrick Bayersdorfer[1], Frederic Timmer[2], Julian Aulbach[1], Henrik Wilkens[2], Lenart Dudy[1], Joachim Wollschläger[2], Ralph Claessen[1], Friedrich Reinert[1], and Jörg Schäfer[1] — [1]Universität Würzburg, D-97074 Würzburg — [2]Universität Osnabrück, D-49076 Osnabrück

Self-assembled nanowires on semiconductors have recently attracted high attention in terms of one-dimensional (1D) physics. The structural confinement on the order of atomic width gives rise to an enhancement of electron correlation effects, leading to exotic many-body phenomena.

As a prototype of 1D metallic chain systems, the Si(111)-(5x2)-Au reconstruction has been widely studied by a variety of spectroscopic and structural techniques. Particularly, it remains unclear whether or not the superstructure relates to a frozen Peierls distortion or to a structural component. However, the definite structural model is still unknown, although it is of vital importance for a precise understanding of the unusual 1D properties in terms of lattice instabilities or correlation physics.

We present a structural investigation of the Si(111)-(5x2)-Au re-

construction by Surface X-Ray Diffraction (SXRD) yielding the two-dimensional Patterson function, as well as several crystal truncation rods. This will be compared with recent theoretical structural models. In addition, we applied spot-profile low-energy electron diffraction (SPA-LEED) to analyse the morphological aspects of this 1D system.

DS 45.7 Thu 16:00 P1

STM study of Dy-induced nanowires on Ge(001) — •Michael Lochner, Robert Bienert, Ulrike Kürpick, and René Matzdorf — Universität Kassel

Quasi one dimensional nanowire structures on semiconductor surfaces are of interest for more than ten years. The scope of this research is the understanding of exotic quantum phenomena like Luttinger-Liquids, Charge-Density-Waves or magnetic ordering in 1D or quasi-1D.

While the atomic structure of Rare Earth metal induced nanowires on silicon surfaces is investigated in many publications, there are less publications on Rare Earth metals on germanium. In this poster, we present our latest STM and LEED data of Dy-induced nanowires on Ge(001).

Similar to Dy-induced nanowires on Si(001), they have different widths, but there is no wetting layer on the Ge(001) surface. The thinnest wires have a width of four Ge lattice constants and their length can vary from just a few to more than 50 nm. We present STM data of the electronic structure in the wires.

DS 45.8 Thu 16:00 P1

Dimensionality and Metallicity of quasi-1D Ag:Si(557) Investigated by Angle-Resolved Photoemission — •Chris Nicholson[1], Claude Monney[1], Ulrich Krieg[2], Michele Puppin[1], Yunpei Deng[1], Christoph Tegenkamp[2], Herbert Pfnür[2], Karsten Horn[1], Ralph Ernstorpher[1], and Martin Wolf[1] — [1]Fritz-Haber-Institut of the Max Planck Society, Berlin, Germany — [2]Leibniz Universität, Hannover, Germany

Self-assembled quasi-one-dimensional (1D) atomic wires on semiconductor surfaces show a range of interesting physical phenomena, and are promising for nanoscale devices. However, the number of metallic systems available is relatively small. Angle-Resolved Photoemission Spectroscopy (ARPES) is a powerful tool that can directly address the metallicity of these systems, and can additionally connect macroscopic conductivity to specific parts of the electronic band structure. We apply ARPES to Ag:Si(557): around 1ML coverage, plasmonic losses with a 1D dispersion have been observed at room temperature in Electron Energy Loss Spectra (EELS), in contrast to insulating behaviour observed with EELS and ARPES at lower Ag coverage. Preparation has been optimised by LEED and ARPES measurements with He I, while high resolution ARPES near the Fermi level allows us to search for metallic surface states and measure their dispersion, in order to assess their relation to the low-dimensional plasmonic excitations. Furthermore, we have developed a new high-repetition rate VUV light source for ultrafast time-resolved ARPES measurements, which will provide complementary dynamic information on such quasi-1D systems.

DS 45.9 Thu 16:00 P1

Evidence of Spin-Orbit Density Waves in Atomic Pb-Wires on Si(557) — •Christian Brand[1], Daniel Lükermann[1], Herbert Pfnür[1], Gabriel Landolt[2], Hugo Dil[2,3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [3]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, Switzerland

Growth of 1.3 monolayers Pb on Si(557) results in a highly anisotropic wire ensemble structure which undergoes a 2D/1D transition when cooling below 78 K as seen by surface sensitive transport measurements. In particular, the system becomes insulating in the direction across the wires. We will show that the mutual interplay between superlattice structures, band filling factors, and spin-orbit coupling results in a highly correlated electronic spin and charge state. By means of spin- and angle-resolved photoemission spectroscopy (SR-ARPES), supplemented by LEED and STM, the spin texture close to the Fermi surface was found to be alternating and equidistant; thus, Fermi nesting occurs in between bands with the same spin texture, giving rise to spin spirals in the direction across the wires. An out-of-phase superposition of both Rashba channels is manifested by an extraordinary large Rashba splitting of $\Delta k_0 = 0.2\,\text{Å}^{-1} = g/2$, where g is a reciprocal lattice vector defined by the interwire distance and fits into the model of spin-orbit density waves in antiferromagnetically ordered chain structures. The implications towards spin-polarized transport along the wires will be discussed.

DS 45.10 Thu 16:00 P1

Spin-Polarization and Spin-Orbit Coupling in Au-Induced Atom Chains on High-Index Silicon Surfaces — •Julian Aulbach[1], Jörg Schäfer[1], Steven C. Erwin[2], Sebastian Meyer[1], Lenart Dudy[1], Bartosz Slomsik[3], Gabriel Landolt[3], Hugo Dil[3], and Ralph Claessen[3] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Germany — [2]Naval Research Laboratory, Washington DC, USA — [3]Paul Scherrer Institut, Villigen, Switzerland

Atoms can form chain-like architectures by self-assembly on various semiconductor surfaces. Such may offer physical realizations of 1D electronic ground states like Peierls instabilities or Tomonaga-Luttinger liquids. Here we report on Au-stabilized nanowires on a high-index silicon substrate, namely Si(553). The two chain types present in that system, one built by Au and one by Si atoms, develop two- and threefold periodicities at low temperatures, which were previously assigned to Peierls instabilities. However, our results from scanning tunneling microscopy and spectroscopy are in astounding agreement with the Si(553)-Au ground state predicted by density-functional theory , where every third Si atom is spin polarized [1]. Moreover, the structural model [2] suggests strong spin-orbit coupling for the Au chains. Using spin- and angle-resolved photoemission we find direct evidence for such a spin-splitting in both Au-induced bands, rendering this system an intriguing 1D material with spin ordering in real and reciprocal space.

[1] J. Aulbach *et al.*, Phys. Rev. Lett. **111**, 137203 (2013).
[2] S. C. Erwin and F. J. Himpsel, Nature Commun. **1**, 58 (2010).

DS 45.11 Thu 16:00 P1

Rashba splitting and relativistic energy shifts in In/Si(111) nanowires — •Nora Jenny Vollmers, Andreas Lücke, Uwe Gerstmann, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, Germany

The electronic properties of quasi-1D systems are of both scientific interest and technological relevance, e.g., for atomic-scale interconnects. The ordered array of In "nanowires" formed upon room temperature (RT) In monolayer deposition on Si(111) substrates and sub-sequent annealing is one of the most intensively investigated model systems in this context. We investigate the influence of relativistic effects, notably the spin-orbit coupling, on the energetics and electronic properties of the In nanowires. Spin-orbit (SO) coupling is well-known to be the driving force behind ferromagnetism und can be used to control the functionality of electronic devices in spintronics. On the other hand, spin-split electron gases may form in asymmetric quantum wells or at surfaces and give rise to the so-called Rashba-(Bychkov) effect even in non-magnetic materials: The break of the spatial symmetry caused by the surface in conjunction with the SO related break of time reversal symmetry lifts the spin degeneracy. Here it is shown that in case of In/Si(111) nanowires – due to an enlarged out-of-plane potential gradient caused by structural anisotropies of the In nanowires – a pronounced splitting of the Rashba type is found at the X point, i.e., at the Brillouin zone boundary.

DS 45.12 Thu 16:00 P1

Raman Spectroscopy of gold-induced nanostructures on plain and high index Si(111) — •Jochen Räthel[1], Eugen Speiser[1], Sandhya Chandola[1], Arne Baumann[1], Norbert Esser[1], Julian Aulbach[2], Sebastian Meyer[2], Utz Bass[2], Martin Liebhaber[2], Lenart Dudy[2], Jean Geurts[2], Jörg Schäfer[2], and Ralph Claessen[2] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Albert-Einstein-Str. 9, 12489 Berlin — [2]Physikalisches Institut and RCCM, Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg

Atomic chains formed by metal adsorption on semiconductor surfaces are used as model systems for determining exotic electronic ground states. Here we present the vibrational properties of Au-induced nanostructures on Si(111) ($(\sqrt{3}\times\sqrt{3})$ and (5×2) phase) and on Si(553) (local (5×2) phase), probed by polarized Raman spectroscopy (RS). Plenty of new surface vibration modes were identified for all three Au related surfaces. By comparing the results from RS of these three Au phases under consideration of different substrates, common structural elements were identified. These results could have a high impact on the verification of theoretical structures models of these systems, e.g., the lowest-energy reconstruction models of Krawiec [1] and the struc-

tural model of Erwin and Himpsel [2]. [1] M. Krawiec, Phys. Rev. B 81, 115436 (2010); [2] S. C. Erwin, Nat Commun 1, 58 (2010)

DS 45.13 Thu 16:00 P1

Optical and electronic properties of gold nanowires on Si(553) — •Sandhya Chandola[1], Eugen Speiser[1], Jochen Räthel[1], Arne Baumann[1], Nobert Esser[1], Conor Hogan[2], Julian Aulbach[3], Sebastian Meyer[3], Jörg Schäfer[3], and Ralph Claessen[3] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert Einstein Strasse 9, 12489 Berlin — [2]Institute for Structure of Matter, National Research Council (CNR-ISM), Rome — [3]Universität Würzburg, Physikalisches Institut, Am Hubland 97074, Würzburg

Reflectance Anisotropy Spectroscopy (RAS) of the clean Si(553), Si(553)-Au and hydrogenated Si(553)-Au surfaces are measured and compared with density functional theory simulations. The lowest energy reconstruction models of Krawiec [1] are used for the calculations of the structure and optical response. Good agreement between experiment and theory is obtained. Local structural elements such as the Si honeycomb chains and the gold atomic wires, which are usually found on gold reconstructed vicinal Si surfaces, yield distinctive features in the optical spectra. By comparing the optical response of the freshly prepared and hydrogenated Si(553)-Au surfaces, the spectral features can be directly attributed to particular structural elements on the surface. Hydrogen adsorption attenuates the anisotropic response at spectral regions associated with the honeycomb chains at the Si step edges and the gold atomic wires. This combination of experiment and theory is very useful in helping to identify specific structural sites on the surface, which generate distinctive features in the optical response. [1] M. Krawiec, Phys. Rev. B **81**, 115436 (2010)

DS 45.14 Thu 16:00 P1

Optical and vibrational characterization of gold-induced atomic wires on germanium (001) — •Jochen Räthel[1], Eugen Speiser[1], Sandhya Chandola[1], Arne Baumann[1], Norbert Esser[1], Utz Bass[2], Jean Geurts[2], Sebastian Meyer[2], Julian Aulbach[2], Lenart Dudy[2], Jörg Schäfer[2], and Ralph Claessen[2] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Albert-Einstein-Str. 9, 12489 Berlin — [2]Physikalisches Institut and RCCM, Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg

Atomic chains formed by metal adsorption on semiconductor surfaces are known as model systems for determining exotic electronic ground states, such as the Tomonaga-Luttinger liquid (TTL). A system of Au-induced atomic wires on the Ge(001) surface has been reported to host such TTL behaviour [1]. Here we present the results of temperature dependent reflection anisotropy spectroscopy (RAS) and Raman spectroscopy (RS) on clean Ge(001) and Au/Ge(001). RAS probes optically surface and surface to bulk electronic transitions between 0.5 and 5 eV with linear polarized light at normal incidence. From polarized RS measurements the vibrational properties of clean Ge(001) and Au/Ge(001) were characterized and in particular surface phonon modes identified. In combination with calculated ab-initio optical and vibrational spectra , the experimental data from RS and RAS provide a basis for structural modeling of these complex surface reconstructions. [1] C. Blumenstein, Nat. Phys. 7, 776 (2011)

DS 45.15 Thu 16:00 P1

Optical properties of gold and indium atom chains on Si(111) — •Fabian Hötzel[1], Olaf Skibbe[1], Eugen Speiser[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]ISAS-Institute for Analytical Sciences, Department Berlin, Berlin, Germany

Optical properties of self-assembled gold atom chains on Si(111) are investigated by Fourier transform infrared spectroscopy in transmittance geometry. Reflection high energy electron diffraction patterns reveal two different domains of 5x2 reconstruction showing metallic behavior between 20 and 423K. Therefore a metal-to-insulator transition of this system can be excluded in this temperature range. The infrared absorption is proportional to the fraction of gold-reconstructed surface and higher at low temperatures. Transmittance spectra can be depicted by a Drude type dielectric function. The resulting sheet conductance is inversely proportional to temperature which emphasizes the metallic character of this system. By means of polarization dependent measurements the orientations of the two domains of gold chains can be identified. Reflectance anisotropy spectra of indium atom chains on the stepped Si(111) surface show an anisotropic interband transition at 1.9eV. The splitting of this feature at 40K along with structural changes of the LEED pattern confirms the metal-to-insulator transition at low temperatures caused by Peierls instability. This contribution is related to DFG-FOR1700.

DS 45.16 Thu 16:00 P1

Optical and electronic properties of rare-earth silicide nanowires on vicinal Si(001) — •Sandhya Chandola[1], Eugen Speiser[1], Stephan Appelfeller[2], Martin Franz[2], Norbert Esser[1], and Mario Dähne[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Berlin — [2]Institut für Festkörperphysik, TU Berlin

Dy and Tb silicide nanowire structures on vicinal Si(001) surfaces are studied using *in-situ* Reflectance Anisotropy Spectroscopy (RAS) and Scanning Tunneling Microscopy (STM). Two different types of structures, metallic nanowires or a wire-like reconstruction, are formed by molecular beam epitaxy depending on the coverage and the annealing temperature. RAS of clean surfaces shows the typical features due to dangling bonds at the steps and Si dimers on the terraces. The silicide growth has a significant effect on the optical anisotropy, e.g. a feature develops at 3.8 eV for both structure types. This peak disappears after the surface is contaminated, confirming that it is unambiguously related to surface state transitions. Furthermore, RAS can identify how well-ordered the metallic nanowires are by the relative magnitude of this peak. The feature of the dangling bonds at the steps is significantly more affected for the wire-like reconstruction than for the metallic nanowires, as supported by the STM data showing that the reconstruction decorates many steps, thereby saturating the dangling bonds. Thus, RAS can be used as an optical fingerprint to distinguish different silicide nanowire structures. This work was supported by the DFG through FOR 1700 projects E2 and E3.

DS 45.17 Thu 16:00 P1

Transport in spatially restricted ensemble wire systems — Frederik Edler, •Stephanie Demuth, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

Low dimensional electron gas systems can be grown by self-organized growth of metals on appropriate semiconducting surfaces. In the recent past various atomic wire structures are found with special properties like Luttinger liquid behavior or Peierls-driven metal insulator phase transitions. Instabilities are directly accessible by surface transport measurements. In order to reveal a deeper insight into the role of coupling of the systems to their environment, transport in spatially restricted areas is highly desirable to correlate imperfections and/or finite size effects directly with transport findings. We have developed a fully in-situ process for Si(111) surfaces to perform such measurements by means of a 4-tip STM/SEM system. For this, oxidation of Si samples is necessary. The SEM e-beam is used to reduce locally the SiO_2 to SiO which is volatile at around 760 °C resulting in Si-windows of arbitrary shape. The subsequent adsorption of 1 ML Ag at 550 °C leads to Ag $\sqrt{3}$-reconstructions only within these windows. Feedback controlled Au-coated W-STM tips are navigated under SEM control for contacting the Ag reconstructions. Transport measurements reveal 2D conductivity of 1.4 kΩ in reasonable agreement with former studies and no contribution of remaining not percolated Ag clusters on SiO_2. We are extending this technique to the In/Si(111) system for a systematically study of finite size effects.

DS 45.18 Thu 16:00 P1

Oxygen Adsorption on the In/Si(111) Nanowire Array: Structure and influence on metal insulator transition — •Stefan Wippermann[1], Duck Mahn Oh[2], Han Woong Yeom[2], and Wolf Gero Schmidt[3] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]Pohang University of Science and Technology — [3]University of Paderborn

The ordered array of In nanowires that self-assembles at the Si(111) surface is an extremely popular model system for one-dimensional (1D) electronic systems. It exhibits an intriguing metal-insulator (MI) transition, that was recently shown to occur as a first order transition starting from condensation nuclei. While the nature of these condensation nuclei remains controversial, Oxygen has recently been observed experimentally to facilitate the metal-insulator transition.

Here we present density functional theory calculations to study the influence of O adsorption on the structural properties and the MI transition of the In/Si(111)-(4x1)/(8x2) nanowire array. We find three different low energy adsorption sites. However, a single oxygen adsorbed at any of these sites does not facilitate the phase transition. Instead,

two oxygen atoms acting in concert catalyze the MI transition by lowering the energy barrier for the formation of 4x2 In hexagons. These in turn act as condensation nuclei for the MI transition.

S. Wall, B. Krenzer, S. Wippermann, S. Sanna, F. Klasing, A. Hanisch-Blicharski, M. Kammler, W. G. Schmidt, M. Horn-von-Hoegen, Phys. Rev. Lett. 109, 186101 (2012)

DS 45.19 Thu 16:00 P1

An Atomistic Picture of Charge Density Wave Formation at Surfaces: Indium Atomic Wires on Si(111) — S. Wall[1], T. Frigge[1], B. Hafke[1], V. Tinnemann[1], B. Krenzer[1], S. Wippermann[2], S. Sanna[2], F. Klasing[1], A. Hanisch-Blicharski[1], W.G. Schmidt[2], and •M. Horn-von Hoegen[1] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Fachbereich Physik, Universität Paderborn

Ultrafast time-resolved reflection high energy electron diffraction was employed to investigate the dynamics of the Peierls-instability-driven phase transition on the (8x2) In/Si(111) surface. At 20 K, far below the critical temperature of 90 K, the (8x2)-(4x1) phase transition is electronically driven through weak excitation with a fs-laser pulse and results in a long-lasting super-cooled excited (4x1) phase. The immediate recovery of the low temperature groundstate is hindered by an activation barrier for the collective motion of the atoms. The recovery of the (8x2) ground state on a timescale of 500 ps is then only triggered by adsorbates that act as nucleation seeds. With increasing density of pre-existing adsorbates the recovery to the groundstate proceeds much faster. The surface unit cells fall back into their ground state one at a time, one-dimensionally like a row of falling dominoes. The phase front propagates at about 100 m/s, comparable to the speed of sound.

DS 45.20 Thu 16:00 P1

Proof of First Order: The (4x2)<>(8x2) Phase Transition in the Indium on Si(111) Atomic Wire system — F. Klasing, T. Frigge, B. Hafke, V. Tinnemann, B. Krenzer, A. Hanisch-Blicharski, and •M. Horn-von Hoegen — Fakultät für Physik, Universität Duisburg-Essen

The In induced (4x1) reconstruction on Si(111) is a prototype for an atomic wire type arrangement of metal atoms on a surface. It has attracted much attention because the In wires undergo a reversible Peierls like phase transition at Tc = 130 K to a (8x2) reconstructed groundstate. In a high resolution LEED study we observed the existence of a robust hysteresis loop upon slow increase and decrease of the sample temperature at Tc. The critical temperatures of the transition are T+c = 135 K and T-c = 125 K for increasing and decreasing temperatures, respectively. The width of the hysteresis loop of 8.6 K is almost independent on the heating and cooling rate and is thus direct evidence for the existence of an energy barrier between the (8x2) ground state and the (4x1) excited state. It unambiguously answers the question about the nature of the phase transition: it is first order.

DS 45.21 Thu 16:00 P1

The conductance phase transition of Si(5 5 7)-Pb probed by Raman and reflectance anisotropy spectroscopy — •Arne Baumann[1], Sandhya Chandola[1], Jochen Räthel[1], Eugen Speiser[1], Daniel Lükermann[2], Christoph Tegenkamp[2], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e. V., Albert-Einstein-Straße 9, 12489 Berlin, Germany — [2]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Germany

Si(5 5 7)-Pb is a model system for a quasi-1D conductor below a phase transition at 78 K, resulting in an anisotropic 2D-phase. The adsorption of 1.31 ML of Pb on the vicinal Si(5 5 7) surface induces a refacetting of the surface into evenly stepped (2 2 3) facets, decorated by wire-like Pb nanostructures. Reflectance anisotropy spectroscopy (RAS) is applied to probe surface band structure transitions and polarized Raman spectroscopy (RS) to characterize vibrational properties.

In RAS measurements the low and high temperature phases exhibit an anisotropic optical conductance behavior and optical transitions in the region between 0.7 and 1.7 eV. This can be assigned to the Pb induced reformation of the surface.

Temperature-dependent RS measurements show new Pb-induced surface phonon modes, while Si-adatom surface vibrational modes persist. A reformation of the terrace structure at 78 K can be excluded. A structural phase transition can only occur on the step edges or between the individual (2 2 3) facets.

DS 45.22 Thu 16:00 P1

Experimental and theoretical evidence for a Peierls insulating state in the low-temperature phase of In/Si(111) — •Eric Jeckelmann[1], Wolf Gero Schmidt[2], Simone Sanna[2], Norbert Esser[3], and Eugen Speiser[3] — [1]Leibniz Universität Hannover — [2]Universität Paderborn — [3]ISAS, Berlin

We reinvestigate the phase transition in indium atomic wires on a Si(111) substrate experimentally with Raman spectroscopy and theoretically using first-principles simulations and model calculations. We construct an effective one-dimensional model for the electronic properties of In wires including a coupling to shear and rotary lattice deformations. Thereby the input parameters for the model calculations are obtained from first-principles frozen-phonon and deformation-potential calculations based on density-functional theory within the local density approximation (DFT-LDA). The present investigation demonstrates that both shear and rotary modes in the low-temperature phase can be interpreted as Peierls lattice deformations which are significantly softened as the temperature increases. This agrees remarkably well with the measured temperature dependence of the surface phonon frequencies in the In/Si(111) atomic wire structure.

DS 45.23 Thu 16:00 P1

HREELS on the In/Si(111)-(4x1) to (8x2) phase transition — •Raphael Müller, Olaf Skibbe, Jan Pischel, and Annemarie Pucci — Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany

Interest in 1D-metallic systems on the nanoscale has increased lately due to interesting properties such as transport anisotropy, charge density waves, Luttinger liquid behavior et cetera.
One example for such systems are self-assembled Indium nanochains on vicinal Si(111) surfaces showing anisotropic collective excitations [1] and a characteristic phase transition whose nature is still under debate [2]. Whilst the In/Si(111)-system was investigated intensively by STM, ARPES and other techniques [3,4], electron energy loss spectroscopy (EELS) with an energy resolution appropriate for surface phonon investigation in the various temperature ranges had not been performed in a comprehensive manner. In order to gain more insight into the reported excitations and the connected phase transition, we used an ELS-22 spectrometer with high energy resolution to probe plasmonic and phononic excitations in the In/Si(111)-nanochains. Here, we report on measurements conducted above and below the phase transition temperature of 120K with excitation parallel and perpendicular to the 1D-metallic chains.

[1] Liu et al., Phys. Rev. B **77**, 205415, 2008.
[2] Wippermann and Schmidt, Phys. Rev. Lett. **105**, 126102, 2010.
[3] Yeom et al., Phys. Rev. Lett. **82**, 4898-4901, 1999.
[4] S. Hasegawa, J. Phys.: Condens. Matter **22**, 084026, 2010.

DS 45.24 Thu 16:00 P1

Tuning of 1d plasmons via selective doping at the edges — •Ulrich Krieg, Timo Lichtenstein, Heiko Teiken, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

We prepared Ag-$\sqrt{3}$ nanowires on the regularly stepped Si(557) surface via self assembly. These wires are of monoatomic height and have an average width of 3.6 nm. Using the intrinsic semiconducting nature of the Ag-$\sqrt{3}$ phase we recently showed that it is possible to tune the 1d plasmon dispersion in a wide range by adsorption of additional silver atoms [1]. This leads to a 1d metallic surface. Using an electron loss spectrometer (EELS) with simultaneous high energy and momentum ($k_{||}$) resolution and SPA-LEED we found strong evidence that the silver doping process is indeed not due to a silver adatom gas, as seen on Ag-$\sqrt{3}$ on Si(111), but due to chemical adsorption of silver atoms at the step edges. This is compatible with the saturation coverage of 0.12ML and the temperature independence of the plasmon energy.

[1] Krieg U, Zhang Y, Tegenkamp C and Pfnür H 2013 *arXiv:1308.5591*

DS 45.25 Thu 16:00 P1

Plasmonic excitations in Au quantum wires on Ge(001) — •Timo Lichtenstein, Heiko Teiken, Christoph Tegenkamp, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung ATMOS, 30167 Hannover

One dimensional electronic systems show exceptional transport properties such as Peierl's transitions or Tomonaga-Luttinger liquid behavior. The latter has been found in Au quantum wires on Ge(001).

Their plasmonic excitations should feature a dispersion relation different from the well-known characteristics in two or three dimensions.

Ge substrate preparation was done ex-situ via chemical etching and in-situ by heating to 900 K in a UHV chamber with a base pressure of 7×10^{-11} mbar. The wires were then formed by evaporation of different amounts of Au at 720 K via self-assembly. The sample quality was controlled with SPA-LEED. Finally, the plasmon dispersion was investigated via EELS combined with a SPA-LEED setup providing both high energy and momentum resolution.

For Au coverages higher than 0.7 ML low-dimensional plasmon modes appear in the loss spectra. Their dispersion relation increases linearly for parallel momentum $k_{||} > 0.1\,\text{Å}^{-1}$, but significantly deviates from the known dispersion of a quasi one-dimensional plasmon for $k_{||} < 0.1\,\text{Å}^{-1}$. A contribution coming from Au clusters seen in SEM can be excluded as the FWHM in the loss spectrum decreases steadily with decreasing $k_{||}$. A dipole excitation can also be ruled out since it would be observable down to zero momentum.

DS 45.26 Thu 16:00 P1

Vibrational properties of Au/Si(553) nanowires — •Sergej Neufeld, Simone Sanna, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

Metallic nanowires on semiconducting substrates such as silicon and germanium have been attracting considerable interest in the last decade. Besides various potential applications as non ohmic conductors, they are candidate systems for the demonstration of the basic concepts of one-dimensional physics such as electron correlation and Luttinger liquid behavior. Furthermore the phase transitions observed on these systems have been controversially discussed and are still poorly understood. Self organizing gold chains at vicinal surfaces such as the Si(553) and Si(557) are of particular interest, as the use of stepped templates allows to vary the geometric parameters and, thus, tune the inter-chain coupling. While well-established microscopic structural models of the Au/Si(553) and Au/Si(557) systems based on density functional theory are available in the literature, few is known about their vibrational properties. In this work, the phonon eigenmodes and eigenfrequencies of the Au/Si(553) wires are calculated from *first-principles* at the center of the Brillouin zone. Several surface localized phonon modes are found, whose phonon frequencies can be directly compared with the spectra obtained by Raman measurements.

DS 45.27 Thu 16:00 P1

Time- and angle-resolved 2PPE studies of Pb nanowires on Si(557) — •Abdul Samad Syed[1], Vesna Mikšić Trontl[1], Manuel Ligges[1], Mathias Sandhofer[1], Ishita Agarwal[1], Isabella Avigo[1], Daniel Lückermann[2], Christoph Tegenkamp[2], Herbert Pfnür[2], and Uwe Bovensiepen[1] — [1]Fakultät für Physik, Univ. Duisburg-Essen — [2]Institut für Festkörperphysik, Leibnitz Univ. Hannover

Strongly anisotropic systems, like, e.g., metallic nanowire arrays grown on semiconducting surfaces, are expected to exhibit significantly different electronic dispersion - along and perpendicular to the wire structure. Angle-resolved photoemission is an excellent tool to study electronic band dispersion, but is often limited to (i) one momentum direction in a single measurement and (ii) the occupied electronic structure. Here, we report on femtosecond-laser based two-photon photoemission experiments on Pb/Si(557) nanowires that map the unoccupied electronic structure. Using a position-sensitive time-of flight spectrometer [1], the dispersion along and perpendicular to the wires can be analyzed simultaneously in a single measurement. Furthermore, by delaying two light pulses with respect to each other, the lifetimes of these unoccupied electronic states can be measured in a pump-probe experiment. We present first time- and momentum-resolved studies on the unoccupied states in this system. We gratefully acknowledge funding by the DFG through FOR1700.

[1] Kirchmann et al., Appl. Phys. A 91,211 (2008)