DS 18: 1D Metal Wires on Semiconductors I (Joint session of DS and O, organized by O)

Time: Tuesday 10:30–13:15 Location: S052

DS 18.1 Tue 10:30 S052

One dimensional plasmons in Si(hhk)-Au — •Timo Lichtenstein[1], Marvin Detert[1], Julian Aulbach[2], Jörg Schäfer[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Physikalisches Institut and RCCM, Universität Würzburg

For future plasmonic devices the understanding of 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. The wire quality was checked with spot profile analysis in low energy electron diffraction (SPA-LEED). A combination of an electron energy loss spectrometer and SPA-LEED providing both high energy and momentum resolution gave access to the plasmon dispersion.

Although 1d metallicity is observed, the plasmon dispersion strongly depends on a two-dimensional crossover: on the lateral distribution of the 1d electron density of states (DOS) within one terrace (intrawire correlation), as well as on the spacing of the wires (interwire correlation). This can quantitatively be described by a modified plasmon model for a wire array. We obtained effective widths of 7.5 Å for Si(553)-Au and 10.2 Å for Si(775)-Au, which are considerably smaller than the terrace widths. A modulated DOS of comparable width can also be seen by tunneling spectroscopy. These effective widths seem to be influenced both by the structural motif, i.e. single or double chain, as well as by the terrace size.

DS 18.2 Tue 10:45 S052

Impurity-mediated early charge density wave condensation in the oxygen-adsorbed In/Si(111)-(4x1)/(8x2) nanowire array — •Stefan Wippermann[1], Andreas Lücke[2], Wolf Gero Schmidt[2], Deok Mahn Oh[3], and Han Woong Yeom[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Universität Paderborn, Germany — [3]Pohang University, South Korea

The self-assembled In/Si(111)-(4x1) nanowire array is an extremely popular model system for one-dimensional electronic systems and features a reversible temperature-induced phase transition into a charge density wave (CDW) ordered ground state. While impurities have been widely known to affect this phase transition, the atomistic mechanisms have rarely been elucidated. Here we present a joint experimental and first principles study, demonstrating oxygen impurity atoms to condense the In/Si(111) nanowire array locally into its CDW ground state, even above the transition temperature. Interestingly, CDW ordering is induced only by a concerted effect of multiple impurities. The mechanism is explained as a subtle interplay between coherent superposition of local impurity-induced lattice strain, a strong coupling between electronic and lattice degrees of freedom, and phononic effects on the free energy. Funding from DFG FOR1700 is gratefully acknowledged.

Invited Talk DS 18.3 Tue 11:00 S052

Taking Nanoscience to the Edge – The Different Appearances of One-Dimensional Physics — •Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

The technologies to fabricate nanostructures on surfaces with atomic precision have become very elaborate, making it possible to play with low-dimensional physical phenomena: among these, approaches to the one-dimensional (1D) world offer a particularly rich arena. What can we expect here? With the lack of effective screening, and in the presence of quasi-1D electron states that promote particular scattering vectors, these systems become susceptible to symmetry-breaking ground states. Idealized examples include, e.g., Peierls instabilities or magnetic ordering – while in real-word systems these phenomena may be far more complex.

The study of such quasi-1D systems on semiconductor surfaces, i.e., atomic wires, has made tremendous progress in the last years. In my talk I will review some of the most interesting realizations. Specifically, I will address the scenarios encountered for multi-band metallic chains with strong spin-orbit coupling, and their tunability. Moreover, as a recent development, we will turn to the step edges of terraced substrates with honeycomb chains, that show strong indications for spin polarization and long-range magnetic ordering. Such setup has intriguing connections to honeycomb topological insulators, predicted to have 1D edge states. The talk will look at this developing field from an overview perspective.

DS 18.4 Tue 11:30 S052

Surface vibrational Raman modes of In/Si(111)-(4x1) and (8x2) nanowires — •Stefan Wippermann[1], Wolf Gero Schmidt[2], Eugen Speiser[3], and Norbert Esser[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Universität Paderborn, Germany — [3]ISAS Berlin, Germany

The ordered array of atomic-scale In nanowires that self-assembles on the Si(111) surface is a prototypical model system for one-dimensional (1D) electronic systems. It exhibits a Peierls-like instability, inducing a reversible phase transition from the metallic (4x1) phase into the insulating (8x2) ground state at $T_C = 120$ K. The detailed nature and mechanism of this metal-insulator (MI) transition is still discussed controversially. We performed a joint *first principles* and surface vibrational Raman spectroscopy study of the In/Si(111)-(4x1)/(8x2) surfaces' vibrational properties. The measured phonons are assigned to characteristic modes of the quasi-1D In nanowires, employing density functional theory calculations and symmetry considerations. Both the (4x1) and (8x2) phases exhibit a distinct set of phonon modes. The observed strong modifications in the Raman spectra of the (8x2) phase are consistent with a symmetric quadrupling of the surface elementary cell and confirm characteristic structural changes at the surface. Funding from DFG FOR1700 is gratefully acknowledged.

DS 18.5 Tue 11:45 S052

Spin correlations in the Si(553)-Au nanowire system — •B. Hafke[1], T. Frigge[1], B. Krenzer[1], J. Aulbach[2], R. Claessen[2], J. Schaeffer[2], and M. Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), 97074 Würzburg

To study the microscopic mechanism of formation, stabilization, and interaction in low dimensional systems we used Si(553) as vicinal surface to enforce the nucleation of Au into one dimensional wires. Deposition of 0.5 ML Au results in the formation of one pair of 1D Au atomic chains per Si terrace exhibiting a twofold periodicity. These metallic wires are structurally terminated by Si step edge atoms, which show a threefold periodicity of the Si atoms along the rows. Theory predicts an antiferromagnetic spin ordering of every third Si step edge atom [1]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in SPA-LEED at a sample temperature of 80 K. The strict twofold periodicity of the Au atoms is not correlated between adjacent wires. In contrast the threefold ordering of the Si spins exhibit a clear short range order perpendicular to the Au wires. Both results support the structure model where the interrow correlation is mediated by the spin-spin interaction of adjacent Si step edge atoms.

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

DS 18.6 Tue 12:00 S052

Interwire coupling of In(4×1) reconstruction probed by transport measurements — •Ilio Miccoli[1], Frederik Edler[1], Stephanie Demuth[1], Herbert Pfnür[1], Stephan Wippermann[2], Andreas Lücke[3], Wolf G. Schmidt[3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Grenzflächenchemie und Oberflächenphysik, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

The In(4×1)/Si(111) reconstruction is used as a prototype for the understanding of 1D systems of atomic chains. It shows strong anisotropic transport properties and a temperature driven metal-insulator transition. Although being intensively studied for more than one decade the effect of defects induced by adsorption (e.g. O_2, H_2) are still under current debate. A better understanding of the influence of defects and a correlation with transport measurements can be achieved by a spatial constriction of the electron path. This restriction was re-

alized by optical ex-situ lithography with reactive ion etching. We report a systematic investigation of the confinement effects using a 4-tip STM/SEM system. Moreover, O_2 adsorption dependent transport studies show not only a reduction of conductivity along the direction of atomic chains but also a decrease in the perpendicular. This was not reported before and reveals an effective interwire coupling between the chains, which is in agreement with recent DFT calculations.

DS 18.7 Tue 12:15 S052

Phase transition of In-Si(111) (4x1)- (8x2) nanowires in a new light — •Eugen Speiser[1], Stefan Wippermann[2], Simone Sanna[3], Wolf Gero Schmidt[3], Sandhya Chandola[1], and Norbert Esser[1] — [1]ISAS e.V., Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

Although recognized as a model case for atomic metallic nanowires, the (4x1)-(8x2) phase transition continues to hide behind the complexity of the structure and electronical properties. In cooperation with continuously developing theoretical methods a variety of conventional and newly developed experimental surface investigation methods are actively applied to elucidate the underlying mechanism of the phase transition. Our approach to this problem is the joint work of calculations and measurements of the low energy surface vibrations localized in the top layer. Successful assignment of calculated vibrational patterns and frequencies to measurements of both the insulating (8x2) and metallic (4x1) phases, is a necessary requirement to understand the dynamics of each phase. Based on this knowledge an interpretation of temperature dependency of phonon frequencies near the phase transition will be given in terms of participation of the electron phonon coupling to the phase transition mechanism. Coupling parameters between phonons and electrons can be estimated from an empirical model based on Landau-Ginsberg theory, as already verified in 1D like bulk materials, eg. blue bronze.

DS 18.8 Tue 12:30 S052

Dynamic Ginzburg-Landau theory for the Peierls transition in In/Si(111) — •Yasemin Ergün and Eric Jeckelmann — Leibniz Universität Hannover, Germany

We investigate thermal fluctuations and collective excitations in quasi-one-dimensional charge-density-wave systems using the Ginzburg-Landau (GL) theory. Starting from a microscopic Su-Schrieffer-Heeger-like model for In/Si(111), we generalized the GL theory for grand canonical Peierls transitions. The equilibrium properties and the non-equilibrium dynamics are simulated using the Langevin approach. We discuss our theoretical results in relation to doping and spectroscopy experiments for In/Si(111). Support from the DFG through the Research Unit FOR 1700 is gratefully acknowledged.

DS 18.9 Tue 12:45 S052

Beyond thermal equilibrium: ultrafast non-thermal melting of a surface CDW in the In/Si(111) atomic-wire system — •Tim Frigge, Bernd Hafke, Tobias Witte, Boris Krenzer, and Michael Horn-von Hoegen — Department of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The wire-type arrangement of Indium atoms on a Silicon(111) surface serves as a famous prototype for the formation of a quasi one-dimensional charge density wave groundstate. We used time-resolved electron diffraction in surface-sensitive geometry to investigate the transient non-equilibrium dynamics of the impulsively driven (8x2)→(4x1) phase transition. Optical excitation of the (8x2) groundstate with fs-laser pulses revealed the existence of a metastable, supercooled (4x1) excited state at 30 K. This phase survives for hundreds of picoseconds because the recovery of the (8x2) phase is hindered due to an energy barrier of 40 meV. At fluences of 3-7 mJ/cm^2 the CDW groundstate is lifted and the structure changes within 350 fs. This photoinduced transition can not be explained by a simple thermal excitation scenario because laser induced heating takes place on timescales 6 times longer. Instead, we explain the observed dynamics through an accelerated displacive excitation scenario upon changes of the potential energy landscape. This also explains the observation of an increase of the excitation time constant towards lower fluences below 3 mJ/cm^2.

DS 18.10 Tue 13:00 S052

Atomistic Mechanism and Dynamics of the Optically Induced In/Si (111) (8x2)-(4x1) Phase Transition — •Andreas Lücke[1], Simone Sanna[1], Uwe Gerstmann[1], Stefan Wippermann[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Interface Chemistry and Surface Engineering Department Max-Planck-Institute for Iron Research GmbH, 40237 Düsseldorf, Germany

The In-Si(111)(8x2)/(4x1) nanowire array features a Peierls instability-driven phase transition, the mechanism of which has been controversial since its discovery, cf. Ref. [1-3]. Experimentally it has been shown that the insulating (8x2) phase undergoes a phase transition towards the metallic (4x1) phase upon optical excitation far below the critical temperature [4]. Here we rationalize this finding by means of ab-initio total-energy and electronic-structure calculations and provide atomistic insight into the driving force and the dynamics of the optically driven phase transition by performing molecular dynamics simulations on excited-state potential energy surfaces. In particular we relate the phase transition to the population/depopulation of specific surface bonds that excite soft phonon modes. Our results rationalize recent findings from ultra-fast time-resolved electron diffraction.

1. H. W. Yeom, et al. Phys. Rev. Lett. 82, 4898 (1999).
2. J. R. Ahn, et al. Phys. Rev. Lett. 93, 106401 (2004).
3. S. Wippermann, et al., Phys. Rev. Lett. 105, 126102 (2010).
4. S. Wall et al., Phys. Rev. Lett. 109, 186101 (2012).