O 90: Poster Session - Semiconductor Substrates: Metallic Nanowires, Overlayers, etc.

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 90.1 Wed 18:15 P2/1OG

Dimerization, self-doping and step-step correlation of Au chains on Si(553) — Zamin Mamiyev, •Priyanka Yogi, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

Adsorption of 0.48 of a monolayer of Au on the regularly stepped Si(553) surface leads to the formation of one double chain of Au per terrace by self-organization. They are considered as a prototype of a quasi one-dimensional system. However, since the interaction with the Si surface results in modifications of the Si surface states, this system turns out not to be purely 1D. In this study we explore the conditions of quasi-1D behavior in more detail by variation of the Au concentration, starting at the optimal concentration of 0.48 ML, as judged from maximum slope and intensity of plasmon dispersion. LEED shows an enhanced coupling between the Au wires at slightly smaller Au concentrations, while a Au surplus up to 0.03 ML adsorbed at RT, dopes the system, removes stacking faults from the wires and simultaneously enhances dimerization, but effectively decouples the wires. By annealing above 630° C the Au atoms are collected in $\sqrt{3}$-ordered clusters with a local concentration of 1ML. Concerning long range order of Au chains, the situation with 0.48 ML Au is restored. The same hold for the plasmon dispersion. Geometric models to explain these properties are discussed.

O 90.2 Wed 18:15 P2/1OG

DFT and ab-inito thermodynamics investigation of $GdSi_2$-nanowires on Si(001) — •Niklas Jöckel[1,2], Kris Holtgrewe[1,2], and Simone Sanna[1,2] — [1]Justus Liebig Universität, Giessen, Germany — [2]Center for Materials Research, Giessen, Germany

In a recent study, detailed STM images of $GdSi_2$-nanowires have been produced[1]. They show a structural connection between the quasi 1D wires and the two-dimensional silicide coverage. On this basis structural models were proposed which we further investigated by ab-initio calculations.

Employing density functional theory, we simulated STM images for different models of two-dimensional silicide layers and compared their stability by minimization of the Landau potential. The two most stable 2D structures that reproduced the experimental STM images were taken as the basis for quasi 1D nanowire models confined to 8 surface lattice constants.

A nanowire structure was found that accurately reproduces the experimental findings. The nanowire is found to be metastable since the system prefers a complete silicide coverage.

[1] Song et al, Sci. Rep. **9**, 1364 (2019)