Grand canonical Peierls transition in In/Si(111): Soft phonons, electronic states and chemical bonds

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Density functional theory calculations on the intensively studied In/Si(111)(4x1)/(8x2) nanowire array are used to illustrate how strongly structural, vibrational and electronic properties of atomic-scale wires are intertwined. Soft phonon modes transform the nanowire structurally between the insulating hexagon structure and metallic In zigzag chains [1]. Starting from a Su-Schrieffer-Heeger-like model inferred from first-principles simulations, it is shown that this metal-insulator transition is a first-order grand canonical Peierls transition in which the substrate acts as an electron reservoir for the wires [2]. This model explains naturally the existence of a metastable metallic phase over a wide temperature range below the critical temperature and the sensitivity of the transition to doping. Also optical excitation changes the potential energy surface of the In nanowires and may melt the charge-density wave far below the critical temperature [3,4]. The femtosecond dynamics of the charge-density wave melting and the picosecond dynamics of the subsequent Peierls condensation is rationalized by ab initio molecular dynamics on ground- and excited-state potential energy surfaces.

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[3] S Wall, S Wippermann, WG Schmidt, M Horn-von Hoegen et al., PRL 109, 186101.
[4] T Frigge, S Wippermann, WG Schmidt, M Horn-von Hoegen et al., PRL 111, 149602.