

Ginzburg-Landau-Langevin theory and SSH model for Peierls transition in In/Si(111)

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Motivated by the thermal and photo-induced first-order Peierls transitions observed in atomic wires on semiconducting surfaces [1], we use the Ginzburg-Landau (GL) theory for charge-density-wave systems to investigate the dynamics of collective excitations in Peierls insulators. This formalism allows us to study the vibrations and the non-equilibrium dynamics of the amplitude modes (lattice distortion and density modulation) which are involved in a Peierls transition. We include no phase mode but amplitude modes for the commensurate Peierls system. The Langevin formalism is used to simulate finite temperature and thermalisation. The GL parameters are determined from the 1D Su-Schrieffer-Heeger (SSH) model in the grand canonical ensemble [2]. Next goals are the extension to coupled chains and the inclusion of non-adiabatic effects between electrons and phonons. Ultimately, we want to simulate the nonequilibrium dynamics of the SSH model for wires on substrates.

References:

[1] M. Horn-von Hoegen et al. PRB 89, 121107(R) (2014).

[2] E. Jeckelmann et al. PRB 93, 241407(R) (2016).