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Graphene on Nickel (100) surface forms a variety of moiré superstructures, due to interfacial lattice parameter and symmetry mismatch. The moiré patterns depend on the misorientation angle and from stripe-like to rhombic-network vary morphology [1]. Physisorbed and chemisorbed regions alternate in stripe-moiré patterns, as shown by combined experimental scanning tunneling microscopy and density functional theory (DFT) simulations. Partial merging of adjacent physisorbed stripes is observed in real samples cooling down the temperature, causing local detachment of graphene from the Nickel surface. The mechanism is investigated with a Kinetic Monte Carlo approach and DFT calculations. which includes surface carbon segregation and local carbide formation.

Evolution of moiré structures of graphene adlayers on Ni(100) surface

Figures

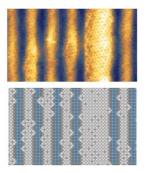


Figure 1: Comparison between STM measurement (top) and Kinetic Monte Carlo simulation (bottom) in presence of carbide segregation for the stripe-like moiré pattern.

References

[1] Zhiyu Z. et al., just accepted by Carbon