Carbide Formation at Graphene/Nickel Interface: The Decisive Role of Graphene Orientation

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When graphene (G) is grown on nickel substrate, the restructuring of the metallic surface upon carbon segregation resulted in the formation of nickel carbide (Ni2C) phase at the interface but solely in rotated graphene (RG) domains and not under the epitaxial graphene (EG) [1]. Motivated by this experimental puzzle, we perform density functional theory calculations to illuminate the microscopic mechanisms governing the structural changes of a C-rich nickel surface under G cover [2]. We show that high concentration of subsurface carbon destabilizes the Ni(111) surface and gives rise to the formation of thermodynamically advantageous Ni2C monolayer. We point out the crucial role of G rotation in enabling high density of favorable C binding sites in nickel subsurface. As opposed to RG, EG cover locks the majority of favorable C binding sites preventing the build-up of subsurface carbon density to a phase transition threshold. In line with strong experimental evidence, we explain why the Ni2C phase formation can take place only if G is misaligned with the Ni(111) surface.

References


Figures

Figure 1: dependence of binding energy of subsurface carbon on the concentration of C atoms at RG/Ni(111) (red) and EG/Ni(111) (blue) interfaces.