Graphene Edges Dictate the Morphology of Nanoparticles during Catalytic Channeling - DTU Orbit (09/01/2019)

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We perform in-situ transmission electron microscopy (TEM) experiments of silver nanoparticles channeling on mono-, bi-, and few-layer graphene and discover that the interactions in the one-dimensional particle–graphene contact line are sufficiently strong so as to dictate the three-dimensional shape of the nanoparticles. We find a characteristic faceted shape in particles channeling along graphene 100 directions that is lost during turning and thus represents a dynamic equilibrium state of the graphene–particle system. We propose a model for the mechanism of zigzag edge formation and an explanation of the rate-limiting step for this process, supported by density functional theory (DFT) calculations, and obtain a good agreement between the DFT-predicted and experimentally obtained activation energies of 0.39 and 0.56 eV, respectively. Understanding the origin of the channels’ orientation and the strong influence of the graphene lattice on the dynamic behavior of the particle morphology could be crucial for obtaining deterministic nanopatterning on the atomic scale.

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