Multicale simulations of the growth of graphene on copper

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Abstract (Arial 10)

In this work, we present simulations of the growth of graphene on copper (111) during chemical vapor deposition (CVD). Basic activation energies for atomic surface diffusion have been obtained by *ab-initio* calculations. We have considered, free atomic diffusion, attachment (detachment) to (from) an island of isolated carbon atom and of carbon atom forming a dimer.
Larger scale growth have been obtained within a four parameters kinetic Monte-Carlo approach. We have considered here atomic diffusion with diffusion barrier depending of the number of first and second neighbors of the initial and final position of the carbon atom. Parameters have been deduced from the *ab-initio* simulations. No defect or surface step in the copper surface are included. We report qualitative results obtained on the size and shape of the islands as a function of growth parameters (temperature and deposition flux). Below, on the left, an example of 'fractal shape' carbon island obtain at T=1273K and high deposition flux (0.1 monolayer/s) and, on the right, the zigzag edge island obtained at same temperature but 0.001 monolayer/s. The dominance of zigzag island edges is reproduced and is explained by its larger dynamical stability, fully present in the model.

Figures