Computer simulation study of the CVD synthesis of carbon nanotubes and graphene

M. Diarra[1, 2], H. Amara [2], F. Ducastelle [2] and C. Bichara [1]

1 Centre Interdisciplinaire de Nanoscience de Marseille – CINaM
CNRS and Aix Marseille University – France
2 Laboratoire d'Etude des Microstructures – LEM – CNRS and ONERA – France

Using the tight binding model developed for nickel and carbon [1, 2] we investigate the growth mechanisms of Single Wall Nanotubes or graphene on a metallic catalyst. In both cases, the solubility of carbon in Ni plays an important role. It favors the growth of SWNT by enabling the nucleation and the dewetting of the tube cap from the catalyst nanoparticle [3-5], but seems detrimental in the growth of graphene, since it makes the control of the structure more difficult (number of layers, in particular). We try and understand the differences in growth conditions and mechanisms by making use of the Grand Canonical Monte Carlo method that is a trademark of our approach.

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