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Multiscale modeling of early stage growth of CNTs produced by a catalytic CVD process JAMES ELLIOTT, University of Cambridge, YASUSHI SHIBUTA, University of Tokyo — The catalytic chemical vapour deposition process is a widely used method for the production of single and multi-wall carbon nanotubes (CNTs), but there remain many uncertainties concerning the precise synthesis mechanisms and therefore the degree of control over the types of CNT that can be produced. Hence, we have developed a parameterized mesoscale model to simulate the early stages of growth of CNTs, and used this to establish a connection between the carbon-catalyst interaction energy, carbon deposition rate and catalyst particle shape and size and the type of CNT produced. The interaction energies for the various components of the model were determined using molecular dynamics simulations [1] using potential functions previously derived from density functional calculations [2] for cobalt, iron and nickel catalyst particles interacting with carbon. We present results from atomistic simulations for the different surface energies of the carbon mesh on various metal nanoparticles, and also influence of additives, such as sulfur or oxygen, on the graphitization ability of transition metals via semi-empirical molecular orbital calculations. [1] Y. Shibuta, J.A. Elliott, *Chem. Phys. Lett.*, **427**, 365-370 (2006). [2] Y. Shibuta and S. Maruyama, *Comp. Mater. Sci.*, **39**, 842-848 (2007).

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