Theoretical model for prediction of metal catalyst in the chemical vapour deposition of carbon nanotubes

ABSTRACT

One of the major challenges in the fields of heterogeneous catalysis and carbon nanotubes (CNTs) synthesis via chemical vapour decomposition (CVD) method is lack of established theoretical model for direct selection of carbon precursor/metal catalyst matrix, which constitutes the most important material parameters of the whole process. In the present report, a theoretical model is proposed via kinetic theory and applied in correlating gas stoichiometry equations and the decomposition of carbon precursors with electrons of metal atoms. Theoretical predictions of this model were found to be in conformity with recent advances in the fields of heterogeneous catalysis in general and CVD synthesis of CNTs in particular. The proposed theory may compliment the current selection of carbon precursor/catalyst matrix through experimental trial and error.

Keyword: Chemical vapour deposition; CNTs; Heterogeneous catalysis; Theoretical model