Simulated PECVD growth of carbon nanotubes: state-of-the-art, challenges and perspectives

E. C. Neyts, A. Bogaerts

University of Antwerp, Research group PLASMANT, Dept. Chemistry, Universiteitsplein 1, 2610 Antwerp, Belgium

erik.neyts@ua.ac.be

Future applications of carbon nanotubes (CNTs) depend to a large extent on our ability to control their exact structure. Plasma enhanced chemical vapor deposition (PECVD) is a possible route towards additional control over the growth process, and thus the CNT structure, compared to traditional CVD growth.

In this contribution, we demonstrate how reactive MD simulations predict and explain PECVD-specific factors influencing CNT nucleation [1, 2]. Specifically, we show how both the electric field and ion bombardment enhance CNT nucleation in a limited parameter window. The electric field is found to allow a lower C-concentration required for the initial nucleation step to take place, and moreover allows vertical alignment of the growing tube. Ion bombardment is – in contrast to general belief – found to actually enhance the nucleation process. These results open new possibilities towards enhanced structural control during the growth process.

Factors contributing to PECVD growth of CNTs [3].