Secteur des Sciences et Technologies

Invitation à la soutenance publique de thèse de

Monsieur Mohammad ZARSHENAS

Master in Physics

Pour l'obtention du grade de Docteur en sciences de l'ingénieur et technologie

« Computational study of acetylene plasme polymerization using molecular dynamics»

qui se déroulera
le lundi 25 mars 2019 à 14h
Auditoire SUD 09
Place Croix du Sud
1348 Louvain-la-Neuve

Membres du jury :

Prof. Arnaud Delcorte (UCLouvain), supervisor
Prof. Tom Leyssens (UCLouvain), supervisor
Prof. Eric Gaigneaux (UCLouvain), chairperson
Prof. Yaroslav Filinchuk (UCLouvain), secretary
Prof. Bartlomiej Czerwinski (Lulea University of Technology, Sweden)
Prof. Erik Neyts (University of Antwerp, Belgium)
Prof. Rony Snyders (Université de Mons, Belgium)

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Plasma polymerization refers to the formation of a polymeric thin film on a substrate under the influence of plasma. Although many experimental results have been reported on the plasma polymerization process and properties of plasma polymer films, the theoretical study of the this process could really help to understand the structure of the formed films and its dependence on various physical parameters. Molecular dynamics (MD) simulations provide an opportunity to investigate the plasma polymerization process at a fundamental level and study the effect of a series of structural parameters on the resulting polymer films. The main goal of this thesis was to model the growth and characterize plasma polymerized acetylene (PPA) films, using computer simulations based on MD. We identified the most proper potential to describe the interaction of hydrocarbons for the formation of PPA films. The REBO potential was found to give the most-realistic energy barrier for the description of the hydrocarbon interactions during the formation of PPA films. We studied the effect of substrate temperature on the growth of PPA film on the Ag(111) substrate. The analysis of the coordination number of carbon atoms shows that the grafting of radicals and molecules on the growing sides of the chains increases with substrate temperature. The investigation of the number of species in the PPA films at each substrate temperature suggests that 300 K is adequate to develop a fully cross-linked structure. Two PPA coatings were developed on nonreactive gold and reactive diamond substrates to investigate the effect of the substrate nature on the growth of PPA films. During the initial stages of deposition, the PPA films grow in a 2D-like manner on gold, in contrast with a 3D growth on the diamond surface. The characterization of the polymerization and crosslinking of the coatings demonstrates that their structures are different in the bulk regions than in the vicinity of the substrates.