Please use the following format for the title of the file so as to ease the management of the web site.

ECXX_LABYY_ NOMChercheur_ Numer
ECXX = ECLi, ECL, ECM, ECN, CS
LABYY = acronyme du laboratoire
NOMChercheur = nom du chercheur émetteur du sujet
Numer = numéro de la proposition (01, 02, é .) pour le chercheur

PhD Proposal 2017

School: CentraleSupelec	
Laboratory: LMSSMAT	**Web site:**
Team: Nanotube and nano/microcomposites	**Head of the team: Jinbo Bai**
Supervisor: Jinbo Bai	**Email: jinbo.bai@centralesupelec.fr**
Collaboration with other partner during this PhD: **In France: Laurent Zimmer (EM2C, CS)**	 **In China:** Prof. Hong-Jian Feng School of Physics Northwest University Xi'an, 710069,China

Title: Atomic simulation of the behaviors of atoms and small nanoparticles during the LII and LIF measurement
Scientific field: Material Sciences
Key words: DFT, LII, LIF, atoms and aggregates, nanoparticles

Details for the subject:

Background, Context:

Carbon nanotubes have attracted huge attention over past decades from academic researchers and industries, due to their specific structures and excellent properties. However, nowadays large-scale controlled production of CNTs is still difficult, and defect-free CNTs are still not available in commercial products, which greatly restrict their industrial applications. A clear understanding of the nucleation and growth processes is crucial to achieve controlled production of high quality CNTs, in which metallic catalyst nanoparticles or clusters play a significant role in a CVD growth process. Although in-situ characterization techniques such LII, LIF and MS can provide some very useful information occurring in the gas phase, a combination with atomic and numerical simulations are highly desired to clearly illustrate the realistic physical and chemical phenomena involved in the catalyst and CNT growth process.

Atomic clusters are the aggregates of a finite number of atoms, and exhibit size-dependent properties. Meanwhile, their chemical and physical properties can vary significantly with atomic composition and ordering.[1] Nanoalloys also display structures and properties which are distinct from those of the pure elemental clusters. Therefore, detailed studies on the clusters by various experimental and theoretical methods can give us a clear understanding of their geometric and electronic structure and physical properties. [2]

In general, we describe nanoallys with a form of AmBn (size m+n, composition m/n). Four main types can be classified four nanoalloys according to their mixing pattern and geometric structure, which contains (a) core-shell segregated nanoalloys, (b) subcluster segregated nanoalloys, (c) mixed A-B nanoalloys, and (d) multi-shell nanoalloys.[3]

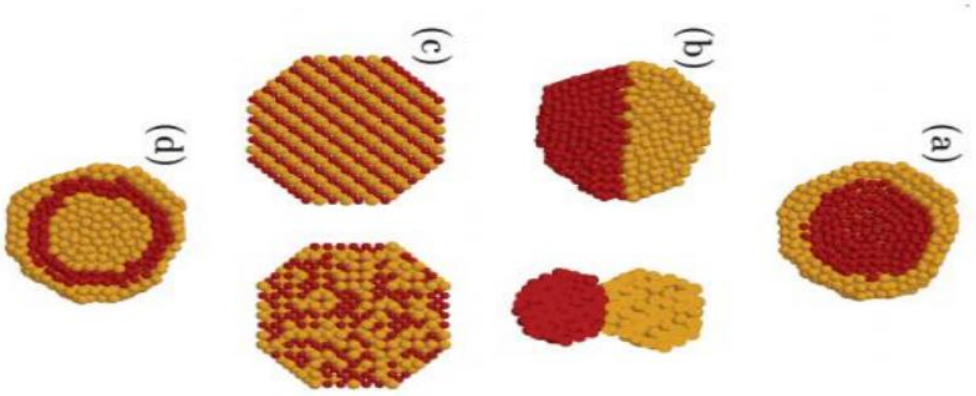

Figure 1：Four types of mixing patterns of nanoalloys.

We can use the theoretical calculation method, such as density functional theory(DFT) and molecular dynamics (MD), to characterize the growth evolution of nanoalloys with the influence of the external environment conditions. The degree of segregation/mixing and atomic ordering in AmBn nanolloys depends on the following factors: (1) relative strengths of A-A, B-B, A-B bonds, (2) surface energy between of bulk element A and B, (3) atomic size, (4) charge transfer, and (5) temperature. [1]

Research subject, work plan:

The main objective of this thesis is to conduct the atomic simulation of the behaviors of atoms and small nanoparticles during the LII and LIF measurement of the CNT growth process.

Computational simulation of the behaviours of atoms will start with building all reasonable models which contain different numbers of atoms.

Then DFT calculation will be performed to select the most stable structure with a lowest energy during optimization process.

After that, we can calculate binding energy to judge the bonding type and the bonding strength, thus to estimate the mixing pattern of AmBn. At the same time, according to the measurement of the chemical bonds damage between molecules, the element with lowest surface energy tends to segregate to the surface according to the lowest energy principle, which can be used to predict the internal distribution patterns of the atoms.

In addition, the ability of attracting electrons between A and B is different due to the distinction of their electronegativity, and the greater electronegativity of an element, the greater tendency to attract electrons it has, which can demonstrate charge transfer in AmBn. [5]

Finally, the temperature is an important factor to influence the internal distribution of the clusters. For large clusters system, molecular dynamics can describe the atomic motion and its internal distribution of cluster under different temperature gradients.

The results of above mentioned theoretical simulation of the behaviours of atoms and small nanoparticles will be analysed in detail, and then compared with the LII and LIF measurements. We can further explore the formation, structure and properties of catalyst clusters during the in-situ synthesis process.

This research is of great significance for researchers to well understand the realistic multiple phenomena involved in catalyst formation, and also to achieve controlled growth of carbon nanotubes. We call for highly motivated candidates who have solid knowledge of materials science, Chemistry, DFT and MD simulation.

References:

[1] Jun-Gang Wang,John S. Fossey, Meng Li,Tao Xie,Yi-Tao Long, Appl. Mater. Interfaces 2016, 8, 8305-8314.

[2]J Sharma,HC Yeh,H Yoo, JH Werner, JS Martinez. Chemical Communications,47(8), 2294-6.

[3] Riccardo Ferrando,Julius Jellinek,Roy L. Johnston. Chemical Reviews, 2008.Vol.108.No.3.

[4] Stenlid J H, Johansson A J, Brinck T. Physical Chemistry Chemical Physics, 2014, 16(6):2452-64.

[5] Makarov G N. Physics-Uspekhi, 2008, 51(4):337ï 376.

[6] Pannier M, Schädler V, Schöps M, et al. Macromolecules, 2000, 33(21):7812-7818