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ELUCIDATING THE CARBON SINGLE WALL NANOTUBE FORMATION: WHERE WE ARE 25 YEARS AFTER THEIR DISCOVERY.

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Carbon multi wall nanotubes (MWNTs) and single wall nanotubes (SWNT) have been identified by S. Ijima in 1991 and 1993 respectively. Although significant progress has been made for 25 years, one major obstacle to realization of SWNTs-based nanotechnology has been the lack of control for designing selective synthesis conditions. This is partly due to the incomplete understanding of the physical and chemical effects driving the kind of tubes able to nucleate and grow under given experimental conditions [1]. In this talk, I will review where we are and our contribution at LEM to this challenging problem.

It is now well established that SWNTs formation mechanism is based on a dissolution – segregation process of carbon at the surface of the metallic nanoparticles [2]. Therefore controlling the state of the particles and their link with the growing tubes is essential for controlling the structure of the tubes. In this context, an enlightening approach is to perform systematic *ex situ* TEM studies of the SWNTs and to inspect their structure, their link with the metal particles and the nanoparticle structure in a statistical way [2, 3]. Thanks to this approach, we have identified two nucleation and growth modes, so- called 'tangential' and 'perpendicular', corresponding to different nanotube-particle junctions [3]. With the support of atomistic simulations [3, 4], we have established and verified with designed specific growth experiments that the growth mode is directly linked with the carbon content of the nanoparticle [5].

A second fruitful approach is to consider SWNT growth from a thermodynamic point of view. To that aim, we have developed a statistical thermodynamics model, which relates the stable tube structures to the tube/catalyst interfacial energies for zigzag and armchair edges and to the temperature [6]. I will show the efficiency of this model in understanding the origin of the frequently reported near-armchair selectivity in perpendicular growth mode [5] and for accounting for observed chirality distributions under given synthesis conditions. Finally the potential of the model will be evaluated for providing guidelines for catalyst design and growth condition optimization

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