In Silico Studies of Carbon Nanotubes and Metal Clusters

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Abstract

Carbon nanotubes have been envisioned to become a very important material in various applications. This is due to the unique properties of carbon nanotubes which can be exploited in applications on length scales spanning from the nano world to our macroscopic world. For example, the electronic properties of carbon nanotubes makes them utterly suitable for nano electronics while the strength of them makes them suitable for reinforcements in plastics. Both of these applications do however require the ability for systematic production of carbon nanotubes with certain properties. This is called selective carbon nanotube growth and today this has not been achieved with total success.

In the work presented in the thesis several different computational methods have been applied in our contribution to the systematic search for selective carbon nanotube growth. Put in a context of previous knowledge about carbon nanotube growth our results provide valuable clues to which parameters that control the carbon nanotube growth. In association with the latest results we even dare to, with all modesty, speculate about a plausible control mechanism.

The studies presented in the thesis addressed different stages of carbon nanotube growth, spanning from the properties affecting the initiation of the growth to the parameters affecting the termination of the growth. In some more detail this included studies of the melting temperatures of nanoscaled metal clusters. The expected size dependence of the melting temperatures was confirmed and the melting temperatures of clusters on substrates were seen to depend both on the material and shape of the surface. As this constitute the premises prior to the carbon nanotube growth it was followed by studies of the interaction between carbon nanotubes and metal clusters of different size and constitution. This was done using different computational methods and at different temperatures. It soon became apparent that the clusters adapted to the carbon nanotube and not *vice versa*. This held true irrespectively of the constitution of the cluster, that is for both pure metal and metal carbide. It was also seen that there exist a minimum cluster size that prevent the carbon nanotube end from closing. Closure of the carbon nanotube end is likely to lead to the termination of the growth which lead to studies of other reasons for growth termination, e.g., Ostwald ripening of the catalyst particles. This was investigated with the result that the rate of the Ostwald ripening may depend on both the chirality and diameter of the carbon nanotubes. It is suggested that this may provide some answers to the controlled growth of carbon nanotubes.

Keywords: Carbon nanotubes, metal clusters, melting temperatures, nanotechnology, molecular dynamics, Monte-Carlo, tight binding, density functional theory.