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Carbon Nanotube Growth on Catalyst

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Abstract: Carbon nanotube (CNT) growth on catalyst as a function of time, temperature, diameter of the CNT, damping factor of the system, and the type of catalyst is investigated via a theoretical analysis on the phonon vibration of the system. Simulations demonstrate that CNTs with larger diameter grow lesser owing to higher damping factors and CNT inertia. In addition, an optimum temperature for the growth is obtained for a CNT with a specific diameter and catalyst. Finally effect of the type of the catalyst on the growth is also discussed. Simulations from the theory are in good agreement with reported experimental results.

Keywords: Carbon nanotube growth, Optimum temperature, Catalyst, Van der Waals bond energy.

1. INTRODUCTION

Carbon nanotubes (CNTs) are macromolecules of carbon in a periodic hexagonal arrangement with a cylindrical shell shape [1]. Their remarkable electrical, mechanical, and thermal properties [2-4], enable them to be used for the development of devices for nanoelectromechanical and nanophotovoltaic system applications [5]. In order to fully optimize the production of CNTs, the growth mechanisms involved in their formation must be completely understood, and a number of theories have been proposed to describe their growth. A mechanism to describe formation of CNTs in the presence of a metal catalyst has been proposed by Sinnott *et al.* [6], which was based on the processes involved in carbon nanofiber formation as described by Baker *et al.* [7-9]. Vaezzadeh *et al.* [10] investigated a theoretical model based on the phonon vibration that simulates the growth of CNT in chemical vapor deposition (CVD) method as a function of time at constant temperature and with a specific catalyst. Li *et al.* [11] showed that controlling the structures of catalytic nanoparticles allows the control of nanotube diameter, and could also enable the control of SWNT length and eventually chirality. Raty *et al.* [12] illustrated that growth occurs from the root by *ab initio* MD simulations of the early stages of SWCNT growth on small iron nanoparticles. Bower *et al.* [13] presented a mechanistic study of the nucleation and growth of aligned nanotubes by microwave plasma CVD. They found that nanotubes grow initially at a very rapid rate followed by a dramatic decrease in its growth. In addition, Gavillet *et al.* [14] investigated root-growth mechanism for single-wall CNTs and showed that the role of the catalyst is not only to stabilize the forming tube but also to provide fluctuating Catalyst-C bonds in the middle of which new carbon atoms are easily incorporated. In view of the experimental and simulation work, a comprehensive study to describe the growth mechanism and reveal the effect of parameter variables, such as the temperature and catalyst, on the CNT growth is indispensable. This paper reports a theoretical model for the oscillation of a CNT on catalyst to provide an investigation on the growth mechanism of CNTs in CVD method. The effect of temperature and type of catalyst on growth process is particularly investigated. Simulations from the theory are in good agreement with reported experimental results.

2. MODELING OF CNT GROWTH ON CATALYST

Owing to the van der Waals bond with catalyst, a CNT oscillates longitudinally on catalyst during its growth. When the distance between CNT and catalyst is more than the diameter of carbon atom, a carbon may involve between the catalyst and tube for a further growth of the tube [10]. It is thus expected the critical amplitude of CNT oscillation, $A_{osc,}$ must be equal to the diameter of carbon atom for a further growth from the current stage. Van der Waals interaction between CNT and its catalyst is simulated by a spring, meanwhile a CNT is simulated by a mass *M(t)* which is increasing during the growth in the theory. Fig. (**1**) is employed to illustrate the phonon vibration of a CNT and its interaction with the catalyst by a spring- mass system.

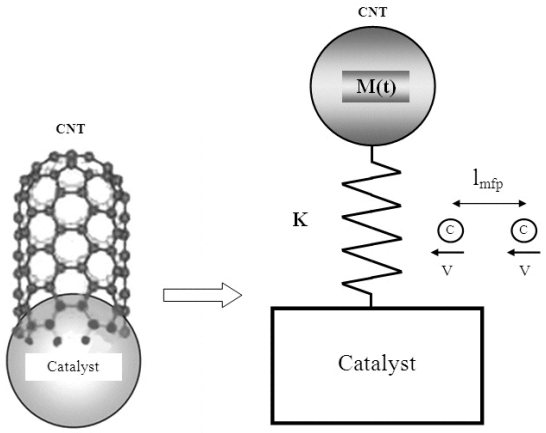

Fig. (1). Model of CNT and its catalyst by a mass - spring system.

The growth of a CNT is described by loops and each loop is made of numbers of carbon atoms *N*. Therefore, the mass of the CNT and the numbers of carbon atoms in one loop are written as,

$$M(t) = n(t)Nm_C \quad \text{and} \quad N = \frac{\pi D}{d_{C-C}}, \tag{1}$$

where $n(t)$, m_C, D and d_{C-C} are number of loops that is increasing during the growth, the mass of a carbon atom, the CNT diameter and carbon- carbon bond length, respectively. Because only the first loop interacts with catalyst, the spring coefficient representing the van der Waals effect, *K,* is provided to be

$$K = Nk, \tag{2}$$

where $k = \frac{2E_{osc}}{A_{osc}^2}$, and E_{osc} and k are energy of oscillation and spring coefficient between a carbon atom and the catalyst, respectively. It is obvious that the number of loops, $n(t)$, is a function of the angular frequency of the oscillation, $\omega(t)$, and time, which is shown in the following expression:

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