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GROWTH OF CARBON NANOTUBES IN LIQUID NANOPARTICLES AND METAL CATALYST SOLUTION

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Abstract:

One of the convenient and cheap methods for growing carbon nanotubes (CNTs) is the catalytic pyrolysis process of acetylene. The growth of carbon nanotubes was studied experimentally. The boundary conditions leading to the separation and encapsulation of the catalyst drop in the inner space of the UNT have been determined.

Keywords: nanoparticles, catalyst, carbon nanotubes, encapsulation

Carbon nanotubes (CNTs) have been one of the most promising and discussed materials in the scientific community since their discovery in 1991. Due to the unique physicochemical properties of UNTs, their fields of application are constantly expanding, including nanoelectronics, composite materials, catalysis, medicine, energy storage, etc. [1–3].

The growth process and properties of carbon structures are significantly influenced by factors such as the composition of the precursor gas mixture, the nature and size of the catalyst particles, the type of substrate, temperature, pressure and duration of the process, etc. Fe, Ni and Co are often used as catalysts for the formation of individual and their mixtures of CNTs, and promoters are added to them. Among the methods of synthesis of carbon nanotubes, there are two main groups: evaporation of graphite at a high temperature of 2700-3700 oC, followed by condensation of steam during cooling, and catalytic pyrolysis of carbon-containing compounds at temperatures not higher than 1000 °C. The second group of methods is the most promising, as it is more suitable for industrial production. [2, 7, 8].

Introduction

The purpose of this work is to determine the factors and conditions that affect the stable position of the catalytic particle on top of the CNT and, as a result, to

determine the stable growth of CNTs during the catalytic pyrolysis of acetylene. There are many publications devoted to the problem of monitoring the growth of CNTs [4-6], many aspects of the growth of CNTs are still insufficiently studied. In particular, the reasons for the often observed instability of the catalyst particles in the upper part of the CNT and their encapsulation in the inner spaces of the nanotubes are not completely clear.

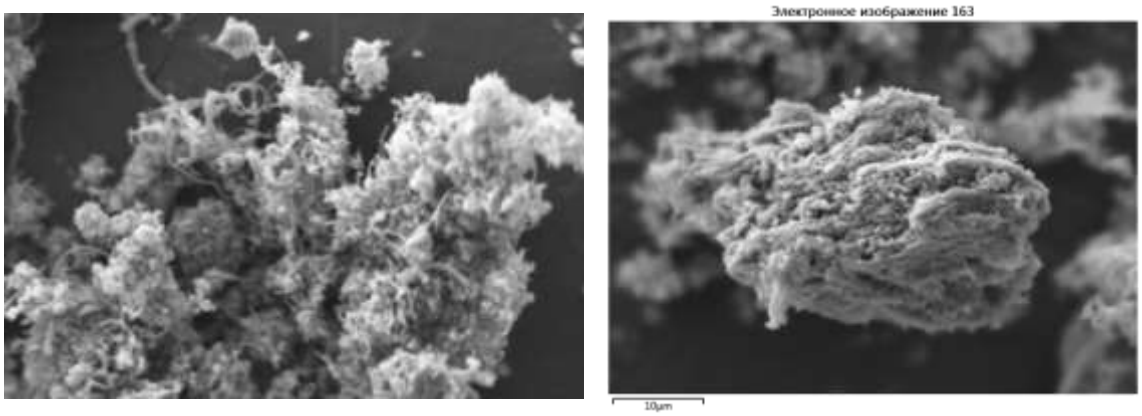
The method of thermal catalytic decomposition of acetylene C_2H_2 was used to synthesize CNTs [6]. To catalyze the growth of CNTs, nanodispersed particles of cobalt chloride (CoCl2) and nickel chloride (NiCl2) obtained by vacuum condensation were deposited on porcelain calcifying boat plates. [8]

Results and discussion

Encapsulation of catalyst particles within nanotubes is typical of all metals we have studied. As the growth temperature of CNTs increased from oC 620 to oC 800, an increase in the number of encapsulated particles inside the nanotubes was observed. Catalyst particles wrapped in nanotubes have an elongated droplet shape. This shape of the encapsulated catalyst particles indicates their liquid phase state during nanotube growth at temperatures between 620 oC and 800 oC.

The mass and structure of CNTs depend on the type of catalyst, process temperature, location of the reaction zone in the reactor, etc.

It is clear that the liquid nanoparticle is a carbon solution in the metal catalyst solution. A drop of a catalyst in mechanical equilibrium at the top of the CNT was considered. The drop of a catalyst located at the top of the CNT is subjected to two opposing forces: the uncompensated force due to the Laplace pressure PL, applied to the opposite part of the droplet surface, and the growth of the droplet CNT (F1) pushes in the direction of [6] Similar to the frictional force, separation of the liquid droplet from the solid surface of the inner cavity of the nanotube (F2) occurs in the region of the back of the moving droplet.



Pic. 1. SEM images of UNTs containing encapsulated particles of nickel chloride and cobalt chloride are shown.

The origin of the F2 force is related to the attraction of the liquid and the solid body on the surface on which it is located by the forces of intermolecular interaction. This interaction can be quantitatively characterized by the energy required to separate the liquid from the solid surface of unit area. Before liquid separation, the energy associated with the liquid-solid interface is equal to αSL per unit area. After the droplet detaches, when it moves in the direction of nanotube growth, two surfaces are formed: one of them is the free surface of the liquid droplet with energy αL, and the other is the free surface of the solid body with energy αS surface. Thus, the release energy of drops falling on a unit area is equal

$$d\alpha=\alpha S + \alpha L - \alpha SL. \quad (1)$$

Whether the drop moves up or breaks depends on the ratio of F1 and F2 forces. For the droplet to break, the following condition must be fulfilled: F1 < F2. When a droplet is broken, a bridge (the narrowed part of the droplet) should form between the main part of the droplet and the small detached droplet. The force F1 pushing up the small drop can be estimated by assigning a certain value to the diameter of the bridge. The diameter of the bridge is equal to the diameter of the nanotube. If R is the radius of curvature of the back of the droplet, r is the inner radius of the nanotube, and the Laplace pressure is PL=2αL/R, then

$$F1= \pi r2PL=2\pi r2\alpha L/R. \quad (2)$$

We find the force F2, considering the drop in contact with the inner surface of the CNT in a circle with a diameter of 2r. Let the drop inside the nanotube move completely through a distance h. In this case, energy consumption (work done) is equal to the product of the value of the area over which the liquid leaves the solid surface.

$$E=2\pi rhd\alpha. \quad (3)$$

Since the work is equal to the product of the force F2 and the distance h,

$$F2=2\pi rd\alpha. \quad (4)$$

Expressing the nanotube radius r as the radius of curvature R of the droplet

$$r=R\sin\theta, \quad (5)$$

where θ is the wetting angle of the droplet.

Considering (2), (4) and (5), we write the condition F1 < F2 as follows

$$\alpha L\sin\theta< d\alpha \quad (6)$$

It follows from the expression (6) that the catalyst droplet on the top of the UNT breaks and leaves the encapsulated liquid-phase inclusions inside the nanotube, if the specific release energy of the droplet is >2αLsina, in this case, the droplet leaving the liquid capsules leaves the solid surface of the nanotube. is more energetically beneficial than opening. We compare the value at with the value of 2aL, because when the droplet breaks off, two surfaces of the liquid are formed. If the value of da is less than 2aLsina, the droplet moves in the direction of nanotube growth without leaving any particles. From the condition da/aL>2sina, the minimum value of the angle a can be found. It can be seen from expressions (1) and (6) that the cracking of the catalyst droplet is favored by good wetting of the carbon nanotube surface with liquid phase catalyst particles, that is, a small angle θ. Better wettability is achieved when UNT growth catalysts such as CoCl2, NiCl2, etc. are used. In order to incorporate any substances into nanotubes, on the contrary, their surface tension should not be higher than 0.2 mJ/m2, which is significantly less than the surface energy of carbon material (~ 2.0-2.5 mJ/m2) and facilitates the process.

Conclusions

The critical condition for the disintegration of the catalyst droplet and the formation of liquid phase inclusions in CNTs is the separation of the droplet from the inner surface of the nanotube, the specific energy of which is twice the free energy. The boundary conditions leading to the decomposition and encapsulation of the catalyst drop in the inner cavity of the CNT are determined. Recommendations are given to ensure the steady state of the droplet during nanotube growth.

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