NANOTUBE FORMATION WITH CONTROLLED PROPERTIES ON CATALYTIC SURFACE BY FULLERENE FLOW

V.I. Maslov, G.A. Skorobagat'ko, A.M. Yegorov, I.N. Onishchenko*
NSC Kharkov Institute of Physics & Technology, Kharkov, Ukraine,
E-mail: vmaslov@kipt.kharkov.ua
**V.N. Karazin Kharkov National University, Kharkov, 61108, Ukraine;*

It has been shown that the bombardment of the nanotubes, growing on the catalytic surface, by fullerenes leads to that if the fullerene molecule kinetic energy exceeds small part of the binding energy of all carbon atoms of the nanotube the nanotube can brake. For convenient further use the nanotubes are oriented in the ordered comb by an electric field. For this purpose the electric field should be more than determined value and it also should be less than other determined value.
PACS: 52.27.Lw

INTRODUCTION

It has been shown theoretically that the bombardment of the growing nanotubes by fullerenes leads in typical conditions to that on the catalytic surface the observed [1] uncontrolled number of twisted nanotubes is formed. Furthermore if the fullerene molecule kinetic energy exceeds 1% of the binding energy of all carbon atoms of the nanotube the nanotube can be braken, as it observed in [1]. For convenient further use the nanotubes are oriented in the ordered comb by an electric field. Thus not number of twisted nanotubes but their oriented comb is formed. For this purpose the electric field should be more than determined value and it also should be less than other determined value. It is determined by that this electric field should not change strongly the kinetic energy of fullerene molecules. These boundary values of the electric field have been determined. At small energies of fullerene molecules the single-wall nanotubes are formed. The mechanism of nanotube filling by fullerene molecules at molecule large energies has been considered. The role of bombardment for the formation of ideal azimuthally symmetrical nanotubes is considered.

CRITERION OF ONE-WALL NANOTUBE BREAK AS A RESULT OF IMPACTS WITH FULLERENES

Let's consider vertically directed nanotube on catalytic surface which is bombarded by fullerenes. Such nanotube tests constant impacts from the fullerenes and as a result to be bent. Nanotube deformation is non-uniformly distributed on its length, and in a point of a break it is maximal. Critical deformation of the nanotube at which it breaks, determined by critical value of displacement of several atoms of its wall, forming cross-section of the nanotube and, taking place in a place of its break. Each such cross-section of the nanotube forms approximately a ring consisting of 12 carbon atoms. At a bend the everyone (i-th) ring turns concerning next on some corner α_i .

Let at fullerene impact with nanotube it is bent in a vertical plane. Then there is some direction (an axis 0x) of displacement from balance position for each atom. We determine x_j displacement of j-th atom in this direction. Then the critical value of such displacement is: $x_{кpj} = x_{кр}$.

Let $\Delta\varepsilon_j$ is the energy of displacement of j-th atom in a nanotube wall as a result of its bend. Then

$$\Delta\varepsilon_j \propto x_j{}^2 \qquad (1)$$

where x_j is the displacement of j-th atom in a nanotube wall in some direction. We enter:

$$U_{ij} = \Delta\varepsilon_j / \Delta S_i \qquad (2)$$

U_{ij} is the energy of displacement of j-th atom of a tube on unit of the area of displacement of i-th rings of the nanotube. I.e. U_{ij} is the energy density of an i-th ring bend of the nanotube, belonging to unit area, passing by this (i-th) ring at its bend concerning the next ring on the corner α_i . Here ΔS_i is the area on a surface of the tube, turning out as a result of displacement of i-th ring of the nanotube. With the account $\varepsilon_{кр} \approx \frac{E_{св}}{3}$ at $x = x_{кр}$ we write down

$$U(x) = \beta x^2 \ , \ \beta = \frac{E_{св}}{3\Delta S_{кр} x_{кр}^2} \ , \qquad (3)$$

where $E_{св}$ is the connection energy of one carbon atom in a nanotube wall, $\Delta S_{кр}$ is the size of the area of displacement of i-th ring at which the nanotube breaks. $x_{кр} = \gamma r_d$, γ <1, r_d is the inter-nuclear distance.

For ΔS_i it is possible to write down:

$$\Delta S_i = 4 \int_0^{\alpha_i} \int_0^{\pi/2} d\varphi \, d\alpha r_f^2 \sin\varphi \sin\alpha \ . \qquad (4)$$

Then

$$\Delta S_{кр} = 4r_f^2 (1 - \cos\alpha_{кр}) \ , \ \sin\alpha_{кр} \approx \frac{x_{кр}}{r_f} \ . \qquad (5)$$

Let's write down

$$\varepsilon_{ki}=\int_{o}^{S_i} dS_i(\alpha,\varphi)U(\alpha,\varphi)= \\ =4r_f^2\int_0^{\alpha_i} d\alpha \int_0^{\pi/2} d\varphi \sin\varphi \sin\alpha U(\alpha,\varphi) \quad . \quad (6)$$

Here $U(\alpha,\varphi)=\beta x^2$; $x=r_f \sin\varphi \sin\alpha$. Then

$$\varepsilon_{ki}=\frac{8}{3}r_f^4\beta\left(\frac{2}{3}-\cos\alpha_i\left(1-\frac{\cos^2\alpha_i}{3}\right)\right) , \quad (7)$$

$$\beta=\frac{E_{св}}{3\Delta S_i x_{кр}^2}=\frac{E_{св}}{12 r_f^2 x_{кр}^2\left(1-\cos\alpha_i\right)} .$$

Full critical energy of a nanotube bend is equal:

$$\varepsilon_{\sum kp}=\sum_{i=1}^{N_k-1}\varepsilon_{ki}= \\ =\frac{2E_{св}}{27\sin^2\alpha_{кр}}\sum_{i=1}^{N_k-1}\frac{\left[2-\cos\alpha_i(3-\cos^2\alpha_i)\right]}{\left(1-\cos\alpha_i\right)} . \quad (8)$$

Let's proceed from the sum on N_k rings to integral on

$$\alpha_i\in\left(\alpha_0;\alpha_{кр}\right): \; d\alpha=\frac{\left(\alpha_{кр}-\alpha_0\right)}{\left(N_k-1\right)}$$

$$\varepsilon_{\sum kp}=\frac{2E_{св}}{27\sin^2\alpha_{кр}}\times ¿ \\ ¿\times\left[\int_{\alpha_0}^{\alpha_{кр}}\frac{\left[2-\cos\alpha(3-\cos^2\alpha)\right]}{\left(1-\cos\alpha\right)}d\alpha\right]\frac{\left(N_k-1\right)}{\left(\alpha_{кр}-\alpha_0\right)} \quad (9)$$

$$¿\frac{E_{св}\left(N_k-1\right)}{27} .$$

The dependence for $\varepsilon_{кр\Sigma}$ can be presented through connection energy $\tilde{E}_{св\Sigma}$ of all nanotube with the fixed N_k . Then for energy of a nanotube break of the fixed length in dependence on its connection full energy in our approximation the following estimation is correct:

$$_{кр}\sum ¿\approx\frac{\tilde{E}_{св}\sum ¿}{162} . \quad (10)$$

$$\varepsilon_{¿} \\ ¿$$

As a result we have derived the dependence of energy of a critical nanotube bend concerning its bend on full connection energy of carbon atoms in nanotube and on quantityof fullerenes from which it was generated.

Let us write down a condition of a nanotube growth without breaks in conditions of their bombardment by fullerenes of environmental plasma. Namely, average kinetic energy of fullerene, falling on nanotube from environmental plasma, is equal $\bar{K}_f=\frac{m_f\bar{v_f^2}}{2}$, where $\bar{v_f}$ is the average fullerene velocity, m_f is its mass. Then for a nanotube formation without breaks the performance of a condition of restriction from above values $\bar{K}_f$ is necessary:

$$\bar{K}_f\le\frac{\varepsilon_{c-c}}{18}\left(\frac{L_{nt}}{r_d}\right) \text{ or } \bar{K}_f\le\frac{\varepsilon_f}{108}\left(\frac{L_{nt}}{d_f}\right) , \quad (11)$$

or $\bar{K}_f\le\frac{\tilde{E}_{св}\sum ¿}{162}$. Here ε_f is the connection energy of all carbon atoms in fullerene, ε_{c-c} is the energy of one carbon - carbon connection, L_{nt} is the length of the nanotube, d_f is the diameter of fullerene.

NANOTUBE STRAIGHTENING IN THE ELECTRIC FIELD

For that the external electric field E_0 orders nanotubes and insignificantly changed kinetic energy of falling fullerenes it should satisfy

$$\frac{2m_f v_f^2}{eN_f L_{nt}\sin^2\alpha_{кр}}<E_0<\frac{m_f\bar{v_f}^2}{eh} ,$$

$\alpha_{кр}$ is the allowable corner of a nanotube deviation; h is the distance, passed by fullerene in the electric field.

REFERENCES

1. G.-H.Jeong, R.Hatakeyama, T.Hirata et al. // *Proc. XXV ICPIG.* Nagoya, 2001, v.2, p.155.

ФОРМИРОВАНИЕ НАНОТРУБОК С КОНТРОЛИРУЕМЫМИ СВОЙСТВАМИ НА КАТАЛИТИЧЕСКОЙ ПОВЕРХНОСТИ ПОТОКОМ ФУЛЛЕРЕНОВ

В.И. Маслов, Г.А. Скоробагатько, А.М. Егоров, И.Н. Онищенко

Показано, что бомбардировка растущих нанотрубок фуллеренами ведет к тому, что, если кинетическая энергия молекулы фуллерена превышает малую часть энергии связи всех атомов углерода нанотрубки, то она может сломаться. Для удобного использования нанотрубок они ориентируются в гребенку электрическим

полем. Для этого электрическое поле должно быть больше определенного значения, но меньше другого значения.

ФОРМУВАННЯ НАНОТРУБОК ІЗ КОНТРОЛЬОВАНИМИ ВЛАСТИВОСТЯМИ НА КАТАЛІТИЧНІЙ ПОВЕРХНІ ПОТОКОМ ФУЛЕРЕНІВ

В.І. Маслов, Г.О. Скоробагатько, О.М. Єгоров, І.М. Онищенко

Показано, що бомбардування фулеренами нанотрубок, що ростуть, веде до того, що якщо кінетична енергія молекули фулерена перевищує малу частину енергії зв'язку всіх атомів вуглецю нанотрубки, то вона може зламатися. Для зручного використання нанотрубок вони орієнтуються в гребінку електричним полем. Для цього електричне поле повинно бути більше визначеного значення, але менше іншого значення.