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Розрахунок площі поверхні наночастинок астралену: Модель

Запропонована модель для оцінки площі поверхні вуглецевих наночастинок поверхня яких складається з структурних елементів різної симетрії. Адекватність моделі перевірено на прикладі розрахунку площі поверхні одностінних вуглецевих нанотрубок. Використовуючи запропоновану модель розраховано площу поверхні та питому площу поверхні наночастинок астралену.

Ключові слова: *площа поверхні, наночастинки, астралени, нанотрубки*

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Evaluation of the surface area of astralene nanoparticles : Model

The proposed model is for the evaluation of surface area of carbon nanoparticles, the surface of this nanoparticles consists of elements with different symmetry types. Adequacy of the model was checked by calculation of surface area of single-wall nanotubes. Surface area and specific surface area of astralene nanoparticles were calculated using this model.

Keywords: *surface area, nanoparticles, astralene, carbon nanotubes*

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The surface area of carbon nanoparticles (carbon nanotubes, fullerenes, actralene etc.) is one of their key properties, which a large extent determines application field of nanoparticles [1]. For example, due to the ultrahigh surface area (SA) carbon nanotubes can be used to produce new generation of electrodes in batteries, and it will reduce battery charging time and increase battery capacity [2]. Also, carbon nanoparticles with ultrahigh SA can be used to create more efficient catalysts that reduce the temperature and the energy required to start the reaction [3]. Examples of other applications of carbon nanoparticles with ultrahigh surface area described in Ref. [4, 5].

With the development of the methods of nanoparticle synthesis appear nanoparticles consisting of elements of different symmetry on significant part of surface, for example, astralene nanoparticles [6]. However, the standard model of calculation of carbon nanoparticles SA is based on calculation of the surface area of the hexagonal cell that make up surface of this nanoparticles [7]. Therefore, standard model can not be applied to calculate SA of carbon nanoparticles with various elements of symmetry on surface.

The aim of this work is the development of model which allows quickly evaluate the surface area of carbon nanoparticles with the surface consisting of elements with different symmetry types. Our model consists in describing of nanoparticle by geometrical figure with the corresponding type of symmetry. For example, carbon nanotubes can be described by a cylinder and astralene nanoparticles by torus (Fig. 1).

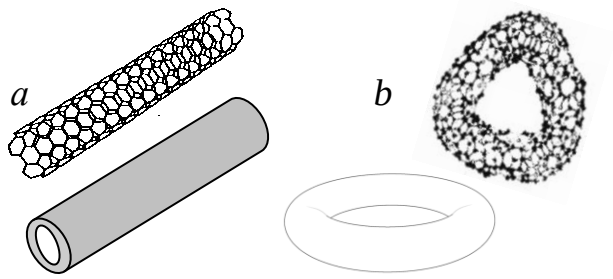

Fig. 1. Schematic representation of carbon nanotube (a), astralene (b) and their models.

Arises logical question: "What is the accuracy of describing the surface area of the carbon nanoparticles using our model?" To answer this question, we calculate the specific surface area of single-walled carbon nanotubes (SSA_{CNT}) using our model. The result of the calculation is comparable to the experimental value (SSA^{exp}_{CNT} = 948 m^2/g) and to the value of the standard model (SSA^{mod}_{CNT} = 1315 m^2/g) [7].

The calculation of SSA_{CNT} was carried out by commonly known formula:

$$SSA_{CNT} = 2\pi R \cdot (l + R) / m$$

where l = 4250 nm and R = 0,747 nm is the length and radius of the carbon nanotube where m = $1{,}5187 \cdot 10^{-17}$ g is the mass of carbon nanotubes with the stated length and radius, calculated using the program Nanotube Modeler. Comparing the calculated value SSA_{CNT} = 1313 m^2/g and SSA^{mod}_{CNT} we see that results of our calculations with the accuracy <0.2% are coinciding with the results of the standard model. However, obtained by us value of SSA_{CNT}, as SSA^{mod}_{CNT}, is slightly larger than SSA^{exp}_{CNT}. This is explained mainly by shortcomings of existing methods of synthesis and purification of carbon nanotubes.

Using the proposed model can calculate the SA and the SSA of astralene nanoparticles. Surface area of astralene SA_{astr} (according to our model astralene by its symmetry is corresponding to geometrical figure torus) was calculated using the formula:

$$SA_{astr} = \pi^2 / 4 \cdot (D^2 - d^2)$$

whetre D and d are the inner and outer diameter of astralene. Results of calculation of SA for modeling nanoparticles of astralene with D from 15 to 180 nm are presented in Fig 2.

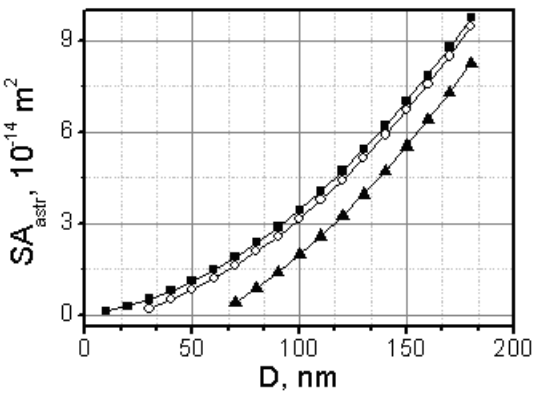

Fig. 2. The dependence of the surface area of astralene nanoparticles of its outer diameter (D). When an internal diameter of astralene: 20 nm (■), 40 nm (○), 80 nm (▲)

SSA_{astr} calculated using the formula:

$$SSA_{astr} = SA_{astr} \cdot (N / M)$$

where M i $N=M/m_{astr}$ – total mass and number of astralene in the sample respectively. m_{astr} – mass of astralene (using Nanotube Modeler). Results of calculation of SSA_{astr} shown in Fig. 3.

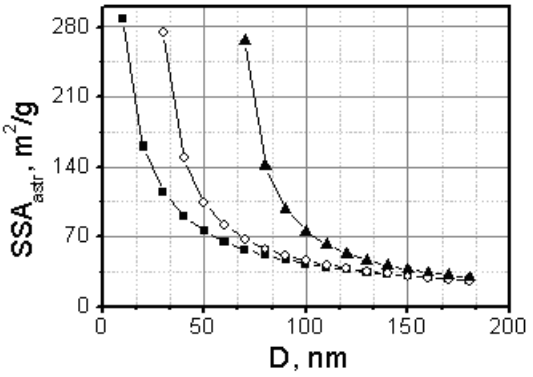

Fig. 3. Dependence of the specific surface area of astralene nanoparticles of their external diameter (D). When an internal diameter of astralene: 20 nm (■), 40 nm (○), 80 nm (▲)

From Fig.2 and Fig.3 we see that SA_{astr} and SSA_{astr} changes with increasing of D for non-linear law. Descending of SSA_{astr} with increasing of D can be explained by the fact that with increasing of D increases the m_{astr} and this dependance predominates over the first one.

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