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The Study Superconductingtheir Fullerene Properties With$_{28}$

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***Abstract* —** *In this paper, based on the fundamental Eliashberg equation, which describes the potential of electron-phonon interaction. a numerical value for the critical temperature of fullerene $C_{28}$is obtained . Examples of the possibility of using fullerenes in various fields of engineering and microelectronics are given.*

Keywords — electron phonon interaction, superconducting fullerenes, nanotubes, nanomaterials, application

One of the main tasks of the directed search for new carbon fullerenes is to establish fundamental dependences of the energy stability of these nanoclusters on their size, topology and composition, based on a detailed study of their electron-energy States. Currently, a large number of model schemes have been proposed and a significant number of quantum chemical calculations of specific fullerenes have been performed, allowing us to link the problem of their stability with the specifics of their electronic structure and the type of interatomic interactions. In particular, the so-called isolated Pentagon rule is proposed, which prohibits the formation of a combination of pentagonal faces separated by an edge [1]. According to this rule, fullerenes with n<60 are unstable, although there is a report of fullerene synthesis With$_{32}$ [2]. Using simple topological methods, the possibility of the existence of a large number of other fullerenes is shown, including the smallest of them - the regular dodecahedron C_{20}. In this connection, the problem of formation of the structure , electronic energy state and stabilization methods of so-called small fullerenes (C_{28}, C_{32}, C_{40}) as “borderline” in the family of cellular carbon nanoclusters is of great interest.

In this paperисследованы сверхпроводя, the superconductingproperties of fullerene $C_{28\ \text{are investigated}}$. The temperature of the superconducting transition, is determined using the electron-phonon interaction potential. The optimized structure of C_{28} is a polyhedron with three groups of nonequivalent C-atoms (Fig. 1) [3]. The upper inhabited non-binding orbitals of C_{28} are localized on four C-atoms, which make up one of the mentioned atomic groups (C1) of the carbon cell.

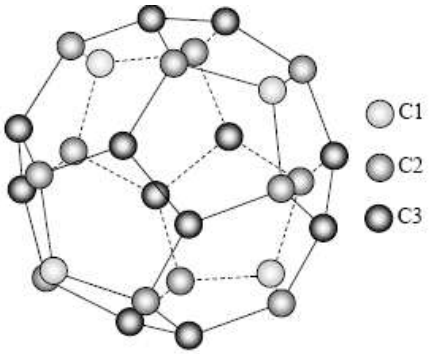

Figure 1. Crystal structure of fullerene C_{28}

As is known [1], under certain conditions, $_{C28\ \text{molecules}}$tend to be ordered in space, they are located in the nodes of the crystal lattice, in other words, fullerene forms a crystal called fullerite. In order for $C_{\text{-28 molecules}}$ to be placed systematically in space, like their atoms, they must communicate with each other. This bond between molecules in a crystal is due to the presence of a weak van der Waals force. This phenomenon is explained by the fact that in an electrically neutral molecule, the negative charge of electrons and the positive charge of the nucleus are dispersed in space, so that the molecules are able to polarize each other, in other words, they lead to a displacement in space of the centers of positive and negative charges, which causes their interaction [3].

To determine the temperature of the superconducting fullerene transition, we will use the well-known Eliashberg equation for the electron-phonon interaction potential [4, 5]

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$$Z(\omega)\Delta(\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{\mathrm{Re}\,\Delta(\omega')}{\omega'} \int_0^{\infty} d\Omega \alpha^2(\Omega) F(\Omega) \times \left[\frac{f(\omega') + N(\Omega)}{\omega' + \Omega - \omega} + \frac{f(\omega') + N(\Omega)}{\omega' - \Omega - \omega} \right] -$$

$$-\mu \int_0^{\varepsilon_F} d\omega' \frac{\mathrm{Re}\,\Delta(\omega')}{\omega'} \tanh \frac{\omega'}{2\tau},$$

$$[1 - Z(\omega)]\omega = \int_0^{\infty} d\omega' \int_0^{\infty} d\Omega \alpha^2(\Omega) F(\Omega) \times \left[\frac{f(\omega') + N(\Omega)}{\omega' + \Omega - \omega} + \frac{f(\omega') + N(\Omega)}{\omega' + \Omega - \omega} \right] +$$

$$\left[\frac{f(\omega') + N(\Omega)}{-\omega' + \Omega + \omega} + \frac{f(\omega') + N(\Omega)}{-\omega' + \Omega - \omega} \right]$$

where Δ(ω) is an order parameter, Z(ω) reshaped function. In the normal state, this function looks like this

$$Z(0) = 1 + \lambda.$$

where λ is the constant of the electron phonon interaction, the function f(ω) and N(ω) – describe the Fermi and Bose distributions, respectively; μ is the matrix element of the Coulomb interelectron interaction, $\alpha^2(\omega)F(\omega)$ – spectral density of the electron-phonon interaction. The matrix element of the electron-phonon interaction was numerically estimated using a finite-differential scheme [5], and it is of the order of ≈ 181 MeV. Using an expression for the electron-phonon interaction constant

$$\lambda = N(0)V_{ep},$$

it is easy to calculate the temperature of the superconducting fullerene transition. As noted in [4], the temperature of the superconducting transition depends on the fullerene lattice constant. The maximum transition temperature of alkali metal fullerenes is slightly higher than 30 K (for example, for a fullerene molecule $With_{60}$), but for a complex composition it exceeds 40 K. Then, according to Macmillan [4]для определения , we use the following expression to determine the temperature of the superconducting transition

$$T_c = \frac{\omega_{\ln}}{1.2} \exp\left[\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right]$$

$$\omega_{\ln} = \frac{2}{\lambda} \int_0^{\infty} d\omega \frac{\alpha^2 F(\omega)}{\omega} \ln \omega \qquad \mu^* = \frac{\mu}{1 + \mu \ln\left(\frac{\varepsilon_F}{\omega_{\ln}} \right)}$$

Here is the phonon frequency, -and here is the Coulomb pseudopotential [6]. Thus, the problem of calculating the temperature of the superconducting transition T_c is reduced to the calculation of the values λ, $\omega_{\ln}$ and μ^*. For typical values of the parameters $\omega_{\ln} = 10^3$ K , λ=1.2 and $\mu^* \approx 0.22$, N(0)=5 eV /spin we have for the temperature of the superconducting fullerene transition $T_c(C_{28}) \approx 8.03 T_c(With_{60}) \approx 200$ K.

Recently, the scientific literature discusses the use of fullerenes for the creation of photodetectors and optoelectronic devices, growth catalysts, diamond and diamond-like films, superconducting materials, as well as as dyes for copiers. Fullerenes are used for the synthesis of metals and alloys with new properties [1]. It was found that fullerenes and nanotubes can form two main classes of condensed phases - molecular and covalently bound.

The first of them are formed with the participation of stable chemically inert nanostructures: nanotubes or higher fullerenes $With_n$. As a rule, the mechanical strength of these phases is low, which is directly related to weak bonds of the van der Waals type between their “building blocks”-fullerenes. The nature of the phenomenon is related to the energy gain during the formation of quasi-plane sections between the outer walls of neighboring nanotubes, which are local fragments of the graphite structure, which contributes to strengthening the connection between neighboring tubes in the beam.This effect can also be achieved under hydrostatic pressure conditions (Fig).

Figure 2. Fullerense nanotubes

Φfullerenes are planned to be used as the basis for battery production. These batteries, whose principle of operation is based on the reaction of hydrogen addition, are in many respects similar to widespread Nickel batteries, but, unlike the latter, have the ability to store about five times the specific amount of hydrogen. In addition, such batteries are characterized by higher efficiency, lower weight, as well as environmental and sanitary safety compared to the most advanced lithium-based batteries in terms of these qualities. Such batteries can be widely used to power personal computers and hearing AIDS [6].

There is a prospect of using fullerenes as a basis for creating a memory environment with ultra-high information density. Fullerenes can be used as additives for rocket fuels and lubricants [7].

Much attention is paid to the problem of using fullerenes in medicine and pharmacology. The idea of creating anti-cancer medicines based on water-soluble endohedral fullerene compounds with radioactive isotopes is discussed. Note that the endeadline compounds, the fullerene molecules, which are placed inside one or more atoms of any element. Conditions for the synthesis of antiviral and anti-cancer drugs based on fullerenes have been found. One of the difficulties in solving these problems is the creation of water-soluble nontoxic fullerene compounds that could be introduced into the human body and delivered by blood to the organ subject to therapeutic action [8].

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