### High-temperature electrical superconductivity of layered nanoscale "heterostructures"

Yu. I. Boyko<sup>1</sup>, V.V. Bogdanov<sup>1</sup>, R. V. Vovk<sup>1</sup>, B. V. Grynyov<sup>2</sup>

<sup>1</sup> V.N. Karazin Kharkiv National University, Svobody square, 4, Kharkiv 61022, Ukraine

<sup>2</sup> Institute of Scintillation Materials of the SSI "Institute of Single Crystals" of the National Academy of Sciences of Ukraine, 60 Nauky Ave., Kharkiv 61072, Ukraine

### Received July 5, 2024

The paper discusses the possibility of realizing a superconducting state at temperatures of  $\approx\!10^2$  K in layered nano-sized heterostructures – thin-film objects consisting of alternating layers of metals and semimetals (or semiconductors) with a thickness of  $(1\!-\!10^2)$  nm. The numerical estimates show that in such structures, an increase in the electron density in semimetals (semiconductors) leads to a change in the electrical conductivity up to the appearance of superconductivity. If we assume that superconductivity is realized as a result of electron-phonon interaction, causing the formation of Cooper electron pairs (Bardeen–Cooper–Schrieffer mechanism), then an increase in the electron density in the semiconductor layer of a nano-sized heterostructure should cause an increase in the pairing constant and so-called high-temperature superconductivity can be realized.

**Keywords**: High-temperature superconductivity, Nano-sized heterostructures, Bardeen-Cooper-Schrieffer mechanism

### Високотемпературна електрична надпровідність шаруватих нанорозмірних "гетероструктур". Ю. І. Бойко 1, В.В. Богданов 1, Р. В. Вовк, Б. В. Гриньов

У роботі обговорюється можливість реалізації надпровідного стану при температурах  $\approx 10^2~\mathrm{K}$  в шаруватих нано-розмірних «гетероструктурах» — тонкоплівкових об'єктах, що складаються з шарів металів і напівметалів (або напівпровідників), що чергуються, товщиною  $(1-10^2)$  нм. Зроблені числові оцінки показують, що у таких структурах відбувається підвищення електронної густини у напівметалах (напівпровідниках), що веде до зміни електропровідності останніх до появи надпровідності. Якщо вважати, що надпровідність реалізується в результаті електрон-фононної взаємодії, що зумовлює формування куперівських пар електронів (механізм Бардіна-Купера-Шриффера), то збільшення густини електронів у напівпровідниковому шарі нано-розмірної «гетероструктури» має зумовити збільшення константи спарювання і може реалізуватися "високотемпературна" надпровідність.

### 1. Introduction

Currently, active research is being conducted into electrical superconductivity (practically zero electrical resistance) of nano-sized structures, that is, objects whose characteristic linear size is  $\approx (1-10^2)$  nm. In particular, superconductivity is realized in samples formed

from thin films of various substances (layered "heterostructures") at the contact of layers of dissimilar metals or contact of metal-semiconductor layers, etc. [1–4]. There is no unambiguous explanation of the microscopic mechanism responsible for the manifestation of this effect in the mentioned objects.

This paper discusses one of the possible reasons for the realization of the superconducting state in nano-sized "heterostructures", the characteristic size of which R (thickness of an individual layer) is comparable with the depth of penetration of electrons into the substance  $\delta$  (shielding length), that is,  $R \approx \delta$ . According to the Thomas-Fermi model, for metals, the value  $\delta$  is  $\leq 1$  nm, and for semiconductors and semimetals,  $\delta \ge 10^2$  nm. At the same time, in our consideration, it is assumed that the main mechanism of superconductivity is the Bardin-Cooper-Shriffer mechanism (the BKS mechanism), based on the idea that superconductivity is realized as a result of electron-phonon interaction, which causes the formation of quantum particles - Cooper pairs of electrons (bosons), capable of carrying an electric charge without loss of energy [5].

# 2. Quantitative assessment of some parameters of the electron energy spectrum in layered nanoscale "heterostructures" with a characteristic size R (layer thickness) comparable to δ (shielding length)

As a simplified model, we will consider a sample of a "heterostructure" containing two layers of different substances: metal-semiconductor or metal-semimetal (non-degenerate semiconductor), which are separated by a thin layer of dielectric with a thickness of  $d \approx 3a$  (a is the crystal lattice parameter of the interlayer substance). As a rule, the dielectric layer is an oxide of the contacting substances.

In the structure under consideration, as a result of a significant difference in electron density in the contacting layers, a redistribution of electrons occurs, leading to the emergence of a contact potential difference U. Obviously the considered model is a flat capacitor. In this case, in the areas adjacent to the interface between the layers, electric charges accumulate, the surface density of which is described by the relation:

$$\sigma = \varepsilon U/d. \tag{1}$$

Here,  $\varepsilon$  is the dielectric constant of the layer that separates the main layers of the heterostructure. Accordingly, the value of the total electric charge arising in each layer is equal to  $q = (\varepsilon U/d)S$ , where S is the area of the interface between the layers of the heterostructure. The appearance of the specified electric

charge causes a change in the electron density  $\Delta n = N/V$  in each layer. Here N = q/e is the number of electrons in the layers due to their redistribution in the heterostructure, e is the charge of an electron, and V is the volume of the layer.

To quantify the relative change in electron density, we use the dimensionless parameter:  $\chi = \Delta n/n_0$ , where  $n_0 \approx 1/\Omega$  is the maximum possible density of free electrons in a substance (metals),  $\Omega$  is the volume of one atom.

Taking into account the above relationship for q, as well as the fact that the volume of the layer V = SR, we have:

$$\chi \approx \varepsilon U \Omega / deR.$$
 (2)

Substituting numerical values of constants into equation (2) and assuming that  $U \approx 1v$  and  $R \approx \delta$ , we obtain:  $\chi \approx 1$  (for a metal layer) and  $\chi \approx 10^{-2}$  (for a semiconductor or semimetal layer).

Thus, the conducted assessments allow us to draw the following conclusions. In layered nano-sized heterostructures, the electron density in metal layers remains virtually unchanged (≈1%). However, in a semiconductor or semimetal layer, despite the small value of the parameter x, the electron density can increase significantly. Indeed,  $n_0 \approx 10^{29}\,\mathrm{m}^{-3}$ , and at  $\chi \approx 10^{-2}$ , we have  $n \approx 10^{27}\,\mathrm{m}^{-3}$ . This is three orders of magnitude higher than the electron density in semiconductors or semimetals in the initial state, i.e. before the formation of a layered nano-sized heterostructure ( $\approx 10^{24} \,\mathrm{m}^{-3}$  [6]). Therefore, there is every reason to state that in the heterostructures under study, electrical conductivity can change significantly, up to the manifestation of the effect of high-temperature superconductivity.

## 3. Estimation of the temperature $T_{\rm c}$ of the transition to the superconducting state of layered nanoscale heterostructures

According to the BKS theory, the temperature  $T_{\rm c}$  of the transition to the superconducting state is described by the following relation:

$$T_c \approx \theta \exp(-1/\mu).$$
 (3)

Here  $\theta$  is the Debye temperature,  $\mu \leq 1$  is the electron pairing constant. For metals and metal alloys  $\theta \approx 300 \,\mathrm{K}$ ,  $\mu \approx (0.1-0.3)$ , so,  $T_{\mathrm{c}} \approx (10-40) \,\mathrm{K}$ , which is in good agreement with the experimental data.

The value of the pairing constant  $\mu$  depends on the density of states  $n^*$  in the energy

spectrum of electrons in the vicinity of the Fermi energy level  $E_{\mathrm{F}}$ :

$$\mu \approx \mathbf{n} \cdot \mathbf{\phi}$$
. (4)

 $\phi$  is the potential of the electron–phonon interaction, which determines the formation of Cooper pairs of electrons.

Using Fermi–Dirac statistics, it is easy to verify that  $n^*\approx N/E_{\rm F}$ , where N is the number of energy states determined by the total number of electrons [7]. Accordingly, taking into account that  $E_{\rm F} \sim n^{2/3} \sim N^{2/3}$ , we have:  $\mu \sim n^{1/3}$ . Therefore, an increase in the electron density in the semiconductor layer of the nano-sized heterostructure by three orders of magnitude should lead to an increase in the pairing constant by approximately 10 times compared to metals, i.e. to reach a value of  $\mu \approx 3$ .

For such values of pairing constant ( $\mu \geq 1$ ) the transition temperature to the superconducting state  $T_{\rm c}$  is described by the following relation [7]:

$$T_c \approx 0.2 \cdot \theta \cdot \mu^{1/2}$$
. (5)

Thus, since the Debye temperature in semiconductors and semimetals is the same order of magnitude as in metals  $\approx\!300\,\mathrm{K}$ , then in the considered version of the layered heterostructure,  $T_{\rm c}$  can reach a value  $\approx\!10^2\,\mathrm{K}$ , which is an order of magnitude greater than in metals, that is, the so-called high-temperature superconductivity can be realized.

Another important aspect of this problem should be noted. In the case of superconductivity by the BKS mechanism, an important parameter is the coherence length, which is interpreted as the size of the Cooper pair. According to various estimates,  $\xi$  is  $\leq 10^2$  nm.

Therefore, in the heterostructures under consideration, superconductivity as a result of the appearance of Cooper pairs (the BKS mechanism) can be realized.

#### 4. Conclusion

Based on the presented assessments and discussion, the following conclusion can be drawn. Nano-sized layered heterostructures formed from contacting "metal-semiconductor" or "metal-semimetal" layers with a characteristic size (layer thickness)  $R \approx 10^2$  nm are capable of realizing a superconducting state at temperatures  $\geq 10^2$  K, which is about 10 times higher than in classical metals. At the same time, the resulting contact potential difference between the layers must reach a value  $\geq 1$  V.

### References

- Bielejec E., Ruan J., Wu W., Phys. Rev. Lett., 87, 3681 (2001).
- Baturina T., Mironov A., Vinokur V., Baklanov M., Strunk C., *Phys. Rev. Lett.*, **99**, 257003 (2007).
- 3. Ohtomo A., Hwang H., *Nature*, **427**, 423 (2004).
- 4. Gozar A., Logvenov G., Kourkoutist L., Bollinger A., Giannuzzi L., Muller D., *Nature*, **455**, 782 (2008).
- Bardeen J., Cooper L., Shrieffer J. Phys. Rev., 108, 1175 (1957).
- 6. Kittel Ch, «Fizika Tverdogo Tela», M., «Nauka», 791 pp. (1978) [in russian].
- 7. Davydov A.S., «Teoriya Tverdogo Tela», M., «Nauka», 689 pp. (1976) [in russian].
- 8. Kresin N., Guttreund H., Little W., Common., **51**, 339 (1984).