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Elastic deformation and anomalous electrical conductivity of semimetals

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The possibility of a significant increase in the electrical conductivity of Group V elements of the periodic table (semimetals) under the action of unilateral compression pressure ≈ 10^{-1} GPa in the area of elastic deformation is discussed. The conditions of such an elastic-stressed state can be realized for nano-sized single-crystal rods ≤ 100 nm in diameter. Under such conditions, the "metallization" of semimetals is possible, leading to a significant change in the energy spectrum of electrons, in particular, to a significant increase in the density of their energy states in the immediate vicinity of the Fermi level. The latter circumstance can cause an increase in the electron pairing constant and facilitate the transition of "metallized" semimetals into a superconducting state at temperatures approaching room temperature. Quantitative estimates are given that confirm the possibility of semimetals "metallization" effect realizing.
Keywords: semi-metals, superconductivity, elastic deformation.

Пружна деформація і аномальна електрична провідність напівметалів. *Ю.І.Бойко, В.В.Богданов, Р.В.Вовк, Б.В.Гриньов*

Обговорюється можливість істотного збільшення електричної провідності елементів V групи таблиці Менделєєва (напівметалів) під тиском одностороннього стиснення ≈ 10^{-1} GPa в області пружної деформації. Умови такого пружно-напруженого стану можуть бути реалізовані для нанорозмірних монокристалічних стрижнів діаметром ≤ 100 нм. За таких умов можлива "металізація" напівметалів, що призводить до істотної зміни енергетичного спектра електронів, зокрема, до значного збільшення густини їх енергетичних станів безпосередньо поблизу рівня Фермі. Остання обставина може зумовити збільшення константи спарювання електронів і сприяти переходу "металізованих" напівметалів до надпровідного стану за температур, що наближаються до кімнатної температури. Наводяться кількісні оцінки, що підтверджують можливість реалізації ефекту "металізації" напівметалів.

Обсуждается возможность существенного увеличения электрической проводимости элементов V группы таблицы Менделеева (полуметаллов) при действии давления одностороннего сжатия ≈ 10^{-1} GPa в области упругой деформации. Условия такого упруго-напряженного состояния могут быть реализованы для нано-размерных монокристаллических стержней диаметром ≤ 100 нм. В таких условиях возможна "металлизация" полуметаллов, приводящая к существенному изменению энергетического спектра электронов, в частности, к значительному увеличению плотности их энергетических состояний непосредственно вблизи уровня Ферми. Последнее обстоятельство может обусловить увеличение константы спаривания электронов и способствовать переходу "металлизированных" полуметаллов в сверхпроводящее состояние при температурах, приближающихся к комнатной температуре. Приводятся количественные оценки, подтверждающие возможность реализации эффекта "металлизации" полуметаллов.

1. Introduction

One of the actual tasks of modern scientific materials science is to study the effect of external pressure on the electrical properties of various substances. A specific important example of this kind of research is the discovery of electrical superconductivity (zero electrical resistance) of metal-hydrogen compounds (hydrides) [1]. So, for example, it was found that the LaH_{10} compound is characterized by zero electrical resistance at temperatures $T \leq 250$ K under the action of uniform pressure $P \approx 150$ GPa [2]. The technical conditions required to create such a significant pressure are very complex, which significantly limits the use of the discovered effect in practice. In this regard, a new problem arose and became urgent — the search for substances that have superconductivity or, at least, increased electrical conductivity under a much lower pressure created according to a simpler scheme and in acceptable technical conditions.

This paper discusses the possibility of a significant increase in the electrical conductivity of the elements of group V of the periodic table (semimetals) under the action of unilateral compression pressure. In this case, we are talking about the pressure at which no phase transformations are observed and plastic deformation of the material is not realized, i.e., it is proposed to use the pressure that causes only elastic (reversible) deformation. The effect under consideration can be conditionally called the effect of "metallization" of semimetals, which causes an abnormal increase in the electrical conductivity of these substances, up to their transition to a superconducting state [3]. It is obvious that the solution of this problem is very important both in scientific and applied terms.

2. The magnitude of the pressure causing the "metallization" of semimetals

One of the possible methods of "metallization" of any substance (dielectric, semiconductor, semimetal) can be realized as a result of collectivization of valence electrons belonging to individual atoms of the substance. In other words, in order to "metallize" a substance, it is necessary to create conditions under which a "gas" of free electrons appears in it. The electron "gas" properties are described exclusively within the framework of quantum mechanics ("gas" of "degenerate" electrons) [4]. Such a state of matter can be realized under the action of external pressure, the value of which is described by the relation

$$P \approx 0.1(h^2/mr^2)n. \qquad (1)$$

Here h is Planck's constant, r is the radius of the orbit of a bound (not collectivized) electron in an atom of matter, m is the mass of an electron, n is the concentration of electrons subject to collectivization [5]. As already indicated, in the case of "metallized" hydrides (dielectrics), this pressure is characterized by a value of the order of $\approx 10^2$ GPa, which corresponds to the concentration of the "gas" of collectivized electrons $n \approx 10^{28}$ 1/m^3. However, semimetals, which include substances such as Bi, Sb, As, etc., in their electrical properties occupy an intermediate position between metals and dielectrics. They are characterized by a slight overlap of the valence and conduction bands, which leads, on the one hand, to the fact that semimetals remain conductors of electricity up to absolute zero temperature, and on the other hand, they are characterized by a low (compared to metals) concentration of charge carriers. So, for example, antimony (Sb), which occupies an average position in this parameter in its group of substances, at room temperature is characterized by the value $n \approx 10^{25}$1/m^3. Thus, in accordance with relation (1), the value of the pressure that can provide the "metallization" of semimetals is $\approx 10^{-1}$ GPa. When using such a pressure according to the unilateral compression scheme, the expected value of the dimensionless elastic deformation $\varepsilon \approx 10^{-1}$ can be estimated using Hooke's law

$$\varepsilon = P/K, \qquad (2)$$

where K is the elastic modulus. For semimetals, the characteristic value of the elastic modulus K in order of magnitude is ≈ 1 GPa and, therefore, the value of the dimensionless elastic deformation under the described conditions should reach the value $\varepsilon \approx 10^{-1}$. However, for conventional samples made of semimetals (polycrystals or single crystals), the elastic deformation region is limited by the values $\varepsilon \leq 10^{-2}$ [3]. This is due to the fact that bulk samples always contain so-called linear defects of the crystal structure (dislocations), the displacement of which causes plastic (irreversible) deformation of the material [6]. In real crystals, the minimum stress at which the dislocations begin to move is usually characterized by the value $P^* \approx 10^{-2}$ GPa (elastic limit) [7, 8]. Thus, while remaining in the elastic region, it is not possible to "metallize" bulk samples made of semimetals and containing dislocations. To carry out the "metallization" of semimetals, it is necessary to use special single-crystal samples in which there are no dislocations. Such objects are ultra-small (nano-sized) single crystals, the diameter of which is ≤ 100 nm [9]. In such samples, due to the action of the so-called "mirror image" force, dislocations under a certain heat treatment move to the crystal surface and there annihilate (disappear) [6]. Obviously, when using single-crystal dislocation-free samples made of semimetals under one-sided compression by pressure $\approx 10^{-1}$ GPa it is possible to achieve the value of elastic deformation $\varepsilon \approx 10^{-1}$ and, therefore, to carry out the "metallization" of these materials without irreversible damage to the structure.

3. Change in electrical conductivity of "metallized" semimetals

As already indicated, semimetals are characterized by a low concentration of electric charge carriers. This circumstance determines the small value of the Fermi energy $\approx 3 \cdot 10^{-2}$ eV in comparison with common metals, for which this parameter is characterized by an interval of values (1÷10) eV. Both of these factors, as well as a slight overlap of the valence and conduction bands, are the reason that the energy spectrum of semimetals can easily undergo significant changes under the influence of various external factors, in particular, under uniaxial compression. In addition to the collectivization of valence electrons described above, i.e., the transformation of electrons into fermions, an increased density of energy states is formed in their energy spectrum in the immediate vicinity of the Fermi level $n_s(E_F)$ [3]. This is indirectly evidenced by the abnormally high values of the dielectric constant of "metallized" semimetals. The changes listed above in the energy spectrum of semimetals that occur under pressure and, in particular, under uniaxial compression, can cause anomalously high electrical conductivity of these substances up to their transition to a superconducting state.

Indeed, according to the quantum theory of superconductivity in metals (BCS theory), the main mechanism of this unique property is the formation of the so-called Cooper electron pairs formed as a result of the electron-phonon interaction [10]. Collectivized electrons (fermions), forming pairs, turn into quantum particles — bosons, which can move in a metal without scattering, i.e. without energy losses. According to the BCS theory, the critical temperature of the transition of a metal to the super-conducting state, i.e., the temperature at which paired electrons are still preserved is generally described by the following relation:

$$T_c \approx \theta \exp\left[-(1+\lambda)/(\lambda - \mu)\right]. \qquad (3)$$

Here θ is the characteristic temperature (Debye temperature), determined by the maximum vibration frequency of atoms (phonons) ν_m: $\theta = (h\nu_m)/k$, h is Planck's constant, k is Boltzmann's constant, λ is the pairing constant ($\lambda \leq 1$), μ is the so-called Coulomb pseudo-potential, which characterizes the mutual repulsion of electrons (usually $\mu \approx 0.1$). In the case of weak electrons pairing, i.e., for $\lambda<1$ and neglecting their mutual repulsion ($\mu \approx 0$), relation (3) transforms to the following form:

$$T_c \approx \theta \exp(-1/\lambda). \qquad (4)$$

For classical metals the Debye temperature is characterized by the range of values (100÷300) K. In accordance with formula (4), for the value of the pairing constant $\lambda \approx 0.3$, the critical temperature of the transition to the superconducting state T_c of classical metals is characterized by the value $\approx (1-30)$ K, which is in good agreement with experimental data [3]. In the case of strong pairing of electrons, i.e., for $\lambda >> 1$, relations (3) and (4) are not applicable, and the critical temperature T_c is described by a different formula [11, 12]:

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

As already indicated, in "metals" obtained under pressure from semimetals, as a result of a significant change in the energy spectrum, the density of energy states ns increases significantly in the immediate vicinity of the Fermi level. This change can provide a significant increase in the pairing constant, since the following relation holds for the pairing constant:

$$\lambda \approx U n_s. \quad (6)$$

Here U is the potential characterizing the electron-phonon interaction.

Obviously, in the case $\lambda >>>1$, the critical temperature of the transition to the superconducting state T_c, in accordance with formula (5), may turn out to be rather high, approaching room temperature. In our opinion, it is this effect that can be realized during elastic deformation $\varepsilon \approx 10^{-1}$ dislocation-free samples obtained from semimetals.

4. Conclusions

Based on the analysis performed and the quantitative estimates made, the following conclusions can be drawn. Nano-sized (≤ 100 nm) samples made of semimetals can be "metallized" according to the uniaxial compression scheme under pressure $\approx 10^{-1}$ GPa and elastic (reversible) deformation $\varepsilon \approx 10^{-1}$. To realize the "metallization" effect, nano-sized single-crystal samples of semimetals should not contain linear structural defects — dislocations. As a result of the semimetals "metallization", a significant change in the energy spectrum occurs in them, in particular, the density of energy states ns increases significantly in the immediate vicinity of the Fermi level. An increase in the density of energy states n_s can cause an increase in the electron pairing constant to values $\lambda > 1$. A significant increase in the pairing constant λ can facilitate the transition of "metallized" semimetals into a superconducting state at temperatures approaching room temperature.

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