Model of superconductivity formation on ideal crystal lattice defect–twin or twin boundary (MSC-TB)

V A Chizhov⁴, F S Zaitsev⁵, V L Bychkov⁶

¹LLC «Processing of energy materials»,
²M.V. Lomonosov Moscow State University,
³NIISI RAS

E-mail: bychvl@gmail.com

Abstract. The report provides a review of the experimental material on superconductivity (SP) accumulated by 2017, a critical analysis of the Bardeen-Cooper-Schrieffer theory (BCS) has been given, and a new model of the superconductivity effect proposed in works of V.A. Chizhov has been presented. The new model allows to understand the mechanism of the SP formation and to explain many experimental facts on the basis of the theory of processes occurring in the ideal defect of the crystal lattice – the twinning boundary (MSC-TB). Specific materials, including new ones, are described, which, in accordance with the theory of MSC-TB, should have improved properties of SC, promising directions for further research are formulated.

1. Introduction

More than 100 years have passed since a discovery of superconductivity (SC) in mercury at a temperature of \( T_c = 4.2 \) K, and a secret of a surprising effect of the SC remains unclear. A confirmation of this is a discovery of high-temperature superconductivity (HTSC) in Cuprate ceramics in 1986: Bednorz and K. Müller, conducting research in the Zurich branch of IBM, found that ceramics based on copper, lanthanum and barium oxide at \( T_c = 30 \) K transforms into a superconducting state. This message shocked the whole scientific world. In 1987, a similar compound of yttrium barium Cuprate showed a transition to the superconducting state above the temperature of liquid nitrogen \( T_c = 92 \) K. New perspectives of superconductivity were opened, since the cost of liquid nitrogen is much cheaper than of liquid helium.

In 2005, the SC was discovered in ferrate-containing compounds – (LaOFeAs) \( T_c = 4 \) K, where nobody expected the appearance of SC, because it was believed that ferromagnetism and superconductivity were incompatible. In 2008, the partial replacement of oxygen O₂ by fluorine F (La\[O_{1-x}Fx\]FeAs (\( x = 0.05\text{–}0.12 \))) led to an increase in the critical temperature by several times \( T_c = 26 \) K. The reason for raising of \( T_c \) remains unclear.

The following superconductivity theories are well known: London’s (1935); Ginzburg-Landau (1950); Bardeen-Cooper-Schrieffer (BCS, 1957). See the bibliography in [1, 2]. By now, the BCS theory is widely accepted. However, none of these theories predicted the experiments on the SC, and cannot fully explain them and predict the origin of the SC in new materials. In fact, all the discoveries of the SC, starting from the very first in 1911, are a matter of chance. The same trend continues to the
present. The search for new superconducting materials is intensively continuing, but there is no systematic approach.

The existing theories of the SC also cannot explain a whole line of experimental facts. The absence of a SC in very good electro-conductive materials (gold, silver, platinum, and copper), and at the same time copper presence in many HTSC compounds – Cuprates. There is no complete description of the Meissner-Openfeld effect mechanism. Only the expulsion of the magnetic field from the volume of the superconductor or levitation – “the coffin of Mohammed” is indicated. However, in reality, in this effect, a levitation of a permanent magnet over a superconductor, and attraction, and a mirror, and memory from a previous exposure to an external magnetic field are observed simultaneously. There is also no understanding of the mechanism of superconductor degradation.

The main reason for the absence of convincing explanations of experiments using the BCS theory is, apparently, non-fulfillment of conditions for the applicability of this theory in reality. The BCS theory was developed for ideal crystals, but it is impossible to use such crystals in experiments. In addition, in the BCS theory, the distances at which Cooper pairs have to interact appear to be much greater than the typical size of the crystal lattice. There are many structural elements of the crystal between the pairs (point donors, acceptors, vacancies, dislocations, small-angle boundaries, twins), but in the BCS theory an effect of such elements on the interaction of pairs is not taken into account.

2. Short description of the model of SC origination on twin boundary MSC-TB

In practice, it is impossible to achieve creation of an ideal crystal without defects. All superconductivity was found in polycrystals. In experiments on SC, one usually works with polycrystals. Polycrystals always have ideal crystal lattice defects-twins or twin boundaries (TB), see Fig. 1-3. Even specially grown high-purity single crystals with SC properties have residual impurity content greater than 1014 cm-3, which can create energy wells of twin boundaries (TB) type.

Let us consider the flow of quasifree electrons of the metallic phase in the TB. We introduce the notation: ΔETB is the energy of the energy well of the twin boundary with respect to the energy of the crystal Ecr; Wke is the kinetic energy of the electron; Eph is the energy of phonons; T is the temperature.

We represent the "work" of the twin boundary in the dynamic mode as ΔETB = ∂ETB / ∂T. The energy of the "well" of the twin boundary |ΔETB| increases with decrease of temperature T and becomes greater than the kinetic energy of the electron Wke. The electron is captured by the "well" and is thrown to the surface, because a direction of movement outwards is more energetically favorable. This action occurs not with one electron, but with all that satisfy the capture condition |ΔETB| ≥ Wke, where Wke = meVd2 / 2, see Fig. 2, 3. One should note an influence of the surface energy Esur on this process, which should allow electrons to "exit" from the TB, i.e. the condition Esur <ΔETB <Ecr has to be satisfied for Esur (for more details, see [1, pp. 37-43]).

Figure 1. A photo of the crystal with the twin boundaries.
Electrons ejected from the TB almost without hindrance go back to the volume of the crystal because of their excessive density above its surface, but under the action of the same TB they are again ejected to the surface.

Thus, in the near-surface layer by means of the TB and its energy well $|\Delta ETB|$ a vortex current is originated, and, consequently, a magnetic field rot $\mathbf{B} = \mathbf{j} + \mathbf{D}/\partial t$, see Fig. 3, 4. The effect of the TB on the electron system in a crystal with lowering of its temperature is described in more detail in [1, p. 55-121].
3. SC effect and the Meissner-Oxenfeld effect
MSC-TB allows to explain many experimental facts [1, 2]. Let us stop here only on a brief explanation of the effect of the SC ("absence" of resistance) and the Meissner-Oxenfeld effect. Let us take into account that there are many twin faces in a polycrystal. Estimates [1, 2] show that for 1 cm\(^2\) there are more than 108 twin boundaries, that is, NTB ≥ 108-1010 cm\(^2\) emission channels for electrons, see Fig. 5.

**Figure 5.** Parameters of electron capture of one TB and estimate of TB density per 1cm\(^2\), \(\bar{a}\) is geometric parameter of the crystal lattice, N is the number of cells in 1 cm of the twin boundary face, \(e^*\) is quasi free electron, \(\mu\) is the electron drift velocity, \(\tau\) is relaxation time, \(n_{TB}\) is the number of electrons captured by TBF during the relaxation time \(\tau\).

If the condition for overlapping of near-surface vortex currents is satisfied at the lowering of the temperature, see, for example, Fig. 15 in [2], and an electric or vortex magnetic field is applied to the crystal, then practically no-obstacle exchange of electrons occurs between the vortices over the TB. The effect of SC takes place, Fig. 6.

The Meissner-Oxenfeld effect in the MSC-TB model is explained by the excitation and orientation of additional vortex currents near the TB when the external magnetic field is applied, which, because of the presence of the TB, flow then for "infinitely" long time. This convincingly explains the properties of levitation, attraction, mirror and memory. More detailed analysis of these effects is presented in [2, p. 18-27].
Conclusion

The proposed model of MSC-TB is based on the analysis of data from all major experiments on SC and uses the most basic physical concepts and laws. There is neither a first-order SC nor the second-order SC, nor a SC of the 1.5-th kind, neither bosons made of electrons nor the polarized phonons. According to the MSC-TB model, in order to obtain the superconductivity effect (SC), it is necessary to create: 1) quasifree electrons of the metal phase type; 2) conduction channels on the crystal surface of the twin-boundary type; 3) the conditions for the capture of electrons into the twin boundaries and their ejection onto the surface; 4) stability of emission channels to degradation. Adequate understanding of the SC mechanism allows predicting superconducting materials with improved properties.

We can formulate what the MSC-TB model predicts for the creation of new SC materials. It is necessary to search for crystals with strong interatomic bonds – they are alkaline-fluoride systems of the type \((d(x) + f(y) + MgF(z-\delta)), \ldots \text{CaF}, \ldots \text{CsF}, \ldots \text{RbF})\) with large lattice period \(\bar{a}\); – in crystals with strong ionic-covalent bond – they are chalcogenides of metals; – in crystals with strong covalent type – such as Diamond.

References

[1] V A Chizhov, Again about superconductivity or experiments are awaiting answers. Moscow: “Sputnik” Publisher. 2015, (in Russian)
[2] V A Chizhov, Again about superconductivity or experiments are awaiting answers. Part II. Moscow: “Sputnik” Publisher 2017, (in Russian)