Calculation of electron transport properties of MgB2 unit cell

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Abstract: As a superconductor material with broad application prospects, MgB2 has received great attention due to its excellent performance and low cost. In this paper, through the description of the superconducting properties of MgB2 and the correlation calculation of its electron transport properties, combined with the density functional theory, the first-principles calculation of the electron transport of MgB2 cells is carried out to achieve the relevant properties.

1. Introduction

MgB2, or magnesium diboride, is known for its unique superconductivity. The mechanism of this superconducting material has been explored and the electronic structure and properties of MgB2 have been studied. The huge research population caused by MgB2 is inseparable from the extensive application prospects of this material. In the review and analysis of relevant literature, the author's current research focus on MgB2 is mainly on its electronic structure, but if it involves the field of electronic transport, it is not good enough. MgB2 is different from general oxide high-temperature superconducting materials. Its particularity determines that in the case of electron transport, if it faces different directions, the properties will change. For example, the optimal transmission direction of superconducting current may exist in this way. In one case, below the critical temperature. In addition, in the field of physical properties, density functional theory has played a significant role in it. Based on this, and also to better analyze the direction of the superconductivity of MgB2, this paper is the experimental work after this article to apply the functional theory, the first principle calculation of the electron transport properties of MgB2 unit cell, for MgB2 the broad application prospects of materials are helping.

2. Overview of MgB2 electronic structure and its superconductivity

2.1 MgB2 electronic structure

The hexagonal structure of AIB2 is the crystal structure of MgB2, which is also commonly referred to as the graphite honeycomb structure in which the B layer is interspersed with hexagonal densely arranged Mg atoms. The research on the electronic structure of MgB2 is mainly carried out from several aspects. The electronic energy band diagram, the second is its density of states, and the third is its charge density, which has made great achievements in related scientific research in these three aspects. As shown in Figure 1, the MgB2 structure forms an ionic bond between magnesium and boron, and the magnesium atom is completely ionized, but this electron is different from other general forms. The boron atom does not completely bind it and move freely in the crystal. It is a place that is different. In addition, it can be found that the powerful dynamics that tie all atoms together are derived from the two-dimensional covalentity existing inside the boron atomic layer, where the two-dimensional covalent bond is a 6-band band due to the 2s orbital and px of the boron atom. The v-orbital is formed by sP2sp hybridization, which is a partially filled energy band and is limited to the boron atomic layer along the I'-K distribution; the three-dimensional metal bond is a two-energy band, originating from the pZ orbital of the boron atom and being non-localized. The distribution along the I'-A, the presence of both electron and hole carrier energy bands and the energy of the two energy bands are very close at the center of the Brillouin, so there can be charge transfer between the two energy bands.

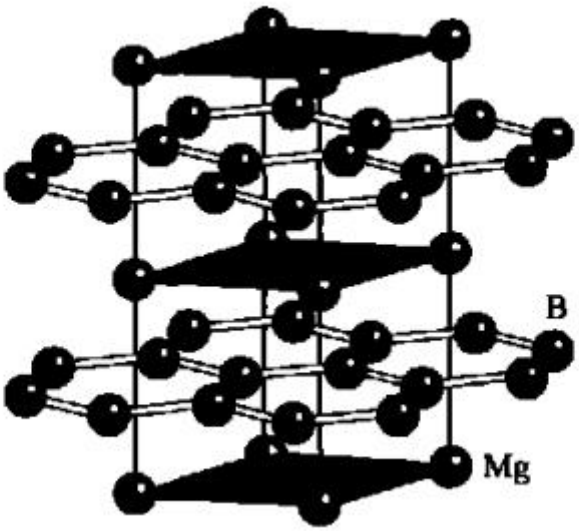

Figure 1 Schematic diagram of MgB2 (magnesium diboride)

2.2 MgB2 superconductivity and its application prospects

The discovery of MgB2 is a great revolution in the field of superconductor research. The breakthrough of change is mainly focused on the superconducting mechanism. It is distinct from the traditional superconductor and belongs to a new class of phonon-mediated BCS superconductors.

The high critical current density of MgB2 determines its wide range of uses as superconducting materials, such as engineering applications, materials research, and related physical applications. Specifically, the analysis of its application is mainly from the following aspects, firstly from the comparison with high-temperature superconductors, and the weak junction of common high-temperature superconductors to destroy the suppression effect of superconducting current transmission, MgB2 The grain boundary does not have such an effect, and its critical current density under high magnetic field is tangibly improved by the strengthening of the magnetic flux pinning center. Secondly, MgB2 is also brilliant in industrial applications, and MgB2 is Its superconducting transition temperature of up to 39K allows people to get rid of the dependence on liquid helium cooling, which means that it has become possible to create a superconducting magnet that is cooled to drive the refrigerator.

2.3 The significance of studying the superconductivity of MgB2

Scientists discovered oxide high-temperature superconductors in 1986, and the myriad of scientific attempts before this made the fact that there were compound superconductors with critical temperatures above 30K. However, the advent of MgB2 broke people's doubts. It brought people a revival of simple compound superconductor research, and it was also a huge push and progress in the development of BCS theory. Nowadays, although the critical temperature of oxide high-temperature superconductors has reached 160K through experiments by researchers, the cost of synthesizing the superconductor is tens or even 100 times that of MgB2, and its popular application is also greatly limited. Because oxide superconductors are difficult to make materials due to their material properties, and MgB2 is the opposite, easy processing is one of its basic attributes. Therefore, the need for low cost and saving social and economic resources has also made a huge impact on the research of MgB2. significance.

3. Inquiry and analysis

We carry out the calculation and analysis of the electron transport of MgB2, using the method of constructing the model. Specifically, we establish a 2-electrode model. The main form can be summarized as the electrode-cell-electricity used in density functional theory. Local density

functional approximation method. Our model uses a parallel structure. The first part is the left and right electrode areas, which are approximated by the ideal crystal structure for the purpose of simplifying the analytical calculation. The second part is the central scattering region, and the analysis of the central scattering region will be This section is expanded below.

In the 2-electrode system of Au-MgB2-Au composed of a MgB2 unit cell and two semi-infinite Au(100) phases, the 2-electrode is an ideal Au(100) crystal structure with a lattice constant of 0.024 nm and a MgB2 unit cell. The structure uses experimental values. In both cases, if the distance between the Mg atomic layer and the 2 electrode is not the same, the analysis process will produce a huge error, so we make a rule that 0.2 nm is between the MgB2 unit cell Mg atomic layer and the 2 electrode. the distance. The transmission spectra of the two structures were calculated. The results are shown in Fig. 2. In the small energy interval near the Fermi surface, the electron transmission coefficient of the c-axis perpendicular to the z-axis is larger than that of the parallel, indicating that the c-axis of the MgB2 unit cell is vertical. On the z-axis, it is more conducive to the transmission of electrons. At zero bias, the equilibrium conductance of the c-axis perpendicular to the z-axis (electron transport direction) is 3.034G0 (G0=2 /h), and the conductance of the c-axis parallel to the z-axis is 1.975G0. In addition, we also calculate the charge transfer amount for the c-axis perpendicular to the z-axis and the c-axis parallel to the z-axis. When the c-axis is perpendicular to the z-axis, the scattering region is 0.042. e,; When the c-axis is parallel to the z-axis, the amount of charge transfer obtained by the scattering region is 0.005e, and it is undoubted that the difference between the two is obvious. We can directly conclude that the amount of charge transferred is larger when the c-axis is perpendicular to the z-axis compared to the amount of transfer of 0.005e parallel to the z-axis of the c-axis, and it is also clear from this that the conductance at this time is very big. Furthermore, we can also conclude that the c-axis is more perpendicular to the z-axis than the parallel case, and the effect on electron transfer and transport is greater.

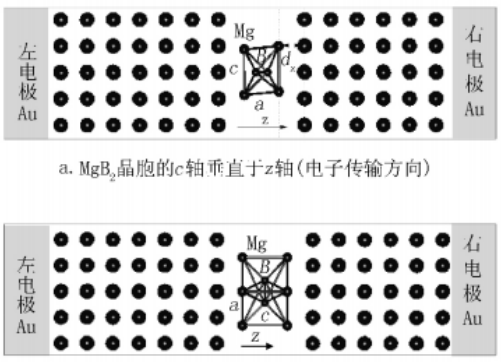

图1 计算模型结构图

Figure 2-1 Model calculation structure

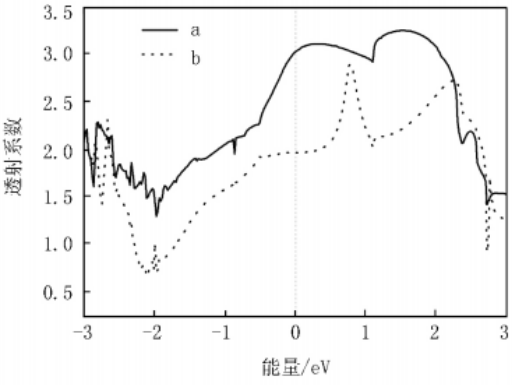

图2 透射谱

Figure 2-2 Transmission spectrum

As shown, the transmission spectra at different voltages are shown. Through the following figure, we can achieve an analysis of the relationship between transmittance and electron energy under different voltage conditions (corresponding to two different structures, respectively). Figure 2-1 shows the transmission spectrum when the c-axis of the MgB2 unit cell is perpendicular to the z-axis (i.e., electron transport direction) at different voltages. The selected voltage range is 0V to 1.2V and is divided into four segments. By observing the figure, the distribution of each curve is roughly the same, the only difference is that when the voltage range is 1.2V, it can be seen that the curve has a significant decrease in the conductance here, which is taken along the curve on the Fermi surface. The value is reduced. Figure 2-2 shows the transmission spectrum at the same selected differential voltage. The only difference is the electron transport direction at this time. The unit cell c-axis is parallel to the z-axis. It can be seen that each curve is highly similar and the conductance is very high. STable, from which we can conclude the inevitability of the existence of a

linear relationship.

4. Conclusion

In this paper, through the selection of the density functional theory tool, the first-principles method is used to calculate the electron transport properties of the MgB2 unit cell. According to the summary and collation of the results, it is concluded that in MgB2, in terms of transmission performance, the effect of electrons in the B atomic layer is better, and this conclusion also reveals a hidden phenomenon, that is, transmission directivity. The presence. The specific first-principles calculation results are: the first one is about the balance conductance, and the value of the axis of the MgB2 unit cell is perpendicular to the z-axis direction is 3.034G0; the second is about the electron transport channel, mainly It is the three channels of B atom, namely px, py, pz orbital; the last is the charge transfer amount, which is 0.042e. At present, the research work of the research frontier in the new superconductor of MgB2 is in full swing. Although it has achieved a lot of achievements, the high-rise building is still not a high-level advanced stage. For example, the exploration of extended intermetallic compound superconductors based on the research of MgB2 is still in progress. To be developed, this article has carried out a small exploration on the electronic transport of MgB2, which still needs to be improved and dig deeper, for reference only.

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