Study on Electronic Structure and Doping of Superconductor Magnesium Diboride

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Abstract: The electronic structure of multi-band dual-gap superconductor magnesium diboride is studied by the linear additive-enhanced plane wave method (LAPW) of density functional theory (DFT). The electron band diagram and density of magnesium diboride are studied. (DOS) and charge density, the electron doping and hole doping of magnesium diboride were studied and analyzed. By replacing the magnesium atom with aluminum atom and replacing the boron atom with carbon atom, the change of charge density is obtained. The changes are explored.

1. Introduction

A superconductor is actually a conductor that has no energy loss after being energized. It is mainly due to the fact that a large number of paired electrons condense into a consistent state in which the crystal is unconstrained and the result of lattice scattering. In 1911, the Dutch scientist Onnes discovered the superconductivity of mercury. This discovery played a key role in the research of superconductivity. Therefore, people have also launched a program to explore superconductors. People’s dream has always been to pursue Room temperature superconductor. With the advent of oxide superconductors, physicists have great interest in this type of superconductor because the superconducting mechanism of oxide superconductors is the most representative superconducting mechanism of the modern era, and this superconductor is more likely to appear in reality. In life, the study of this superconducting mechanism is of great significance and challenge. The interaction between the electrons of the oxide superconductor is very strong. Using the original knowledge of solid physics to analyze the motion behavior of the electron can not be supported. Therefore, from the high-temperature superconductor, the mechanism of the high-temperature superconductor is learned, and the strong correlation with the electron is obtained. The study of the physical nature of materials. Realize the all-round development of science and technology.

Since 2001, the superconductivity of magnesium diboride has been the focus of physicists. The main reason is that the critical temperature of magnesium diboride can reach 39K, which appears on the simple binary alloy superconductor. It is very unusual, and it is also the case, which has aroused people's strong concern, and quickly carried out research work on magnesium diboride. It has been found through research that the superconductor can carry an ultra-high superconducting current at a temperature of about 20K and 80,000 times the earth's magnetic field, but the energy consumption is extremely low. Moreover, the temperature of 20K can be obtained by a small refrigerator, so the application range of this kind of superconductor will be very extensive, and it has a great help to improve the superconducting magnet of the hospital nuclear magnetic imaging instrument, by replacing the original expensive liquid helium with two. Magnesium borate will greatly reduce the cost of the hospital. The price of magnesium diboride material is not high, and it is easier to process than ceramic high-temperature oxide superconductors. So after a short discovery, a laboratory in the United States can stretch out tens of meters of such materials. The superconducting coherence length of the magnesium diboride superconductor is long, so this characteristic can be used to produce a superconducting quantum interference device, which is used for the detection of electromagnetic signals and promotes the development of medical instruments, environment and military in China.

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2. Basic characteristics of magnesium diboride

2.1 Crystal structure of magnesium diboride

The crystal structure of magnesium diboride (MgB2) is a hexagonal structure of type A1B2. As shown in Fig. 1, it is composed of a hexagonal densely arranged Mg atom interposed between the B layers of the graphite honeycomb structure, and the space group is P6/mmm. The lattice parameters obtained by X-ray and structural analysis were a = 3.086 A, c = 3.524 A. The Mg and B atoms occupy positions 1a and 2d, respectively, and each solid physics element contains a formal structural unit (Z = 1).

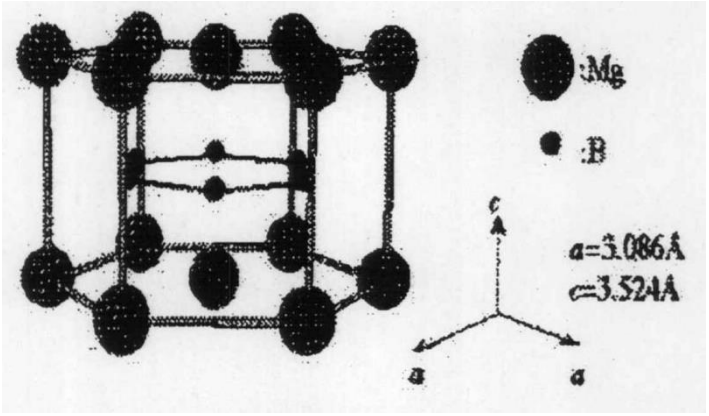

Figure 1 Magnesium diboride crystal structure

2.2 Electronic structure of magnesium diboride

Theoretical studies have shown that the substantially fully ionized Mg, the energy band structure at the Fermi level is mostly derived from the plane wage bond of B, B, and the B-Mg particle bond extending outward from the B plane. Thereby exhibiting sp-type metal characteristics of MgB2. The charge is transferred out of the B plane in the B plane, leaving hole carriers in the B plane. It is precisely because the hole carriers interact with the phonons in the B plane that the MgB2 has an ultrahigh superconducting transition. temperature. Moreover, the superconductivity of MgB2 is mainly derived from the metallicity of the 2D shell of B. Since the boron atoms have different weights, the high vibration frequency of the lighter boron atoms results in the high Tc of the MgB2 superconductor. MgB2 has two different S-wave superconducting energy gaps, which correspond to two different branches of the Fermi surface. The shape of the Fermi surface is shown in Fig. 2. The superconducting properties of MgB2 have been verified by theory and experiment.

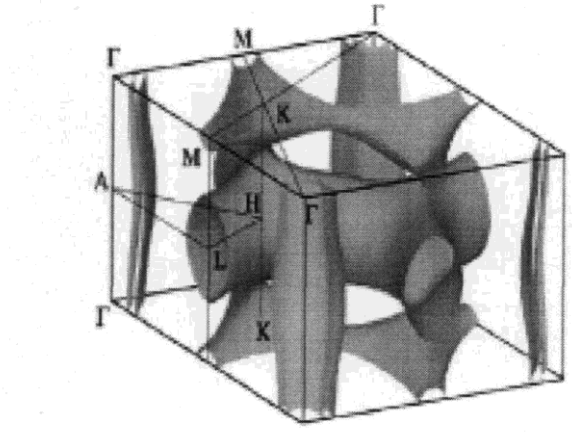

Figure 2 Fermi surface structure of magnesium diboride

2.3 Characteristics of superconductivity of magnesium diboride

The superconducting mechanism of magnesium diboride is a phonon-mediated BCS superconductor. This kind of superconducting mechanism is only one kind of superconducting

mechanism, and there are even many strange superconductors. Experimental studies have shown that the superconductivity of magnesium diboride is determined by the phonon spectrum of boron atoms, so it can be known why magnesium diboride is a phonon-mediated BCS superconductor. This conclusion can be proved even by other experiments. We often say that the critical temperature decreases with the increase of pressure. By using different methods to verify, it is found that phonons play a dominant role. Whether it is high temperature or low temperature, the results are basically the same, and then One problem that comes up is that magnesium diboride can continue to carry a large superconducting current when there is a large magnetic field in the outside world. As far as the current oxide high-temperature superconductors are concerned, they are faced with the influence of uncertain factors in reality, so sometimes it is impossible to provide such comprehensive protection, so that the weak connection between the grain boundaries in the polycrystalline sample leads to diboron. The superconducting flow carrying capacity of magnesium has decreased. Although magnesium diboride has a high critical temperature value, it still cannot get rid of the weak connection. The superconducting flow density of magnesium diboride is high, and the superconducting current is not affected by the grain boundary connection. However, the superconducting current of magnesium diboride is inversely proportional to the magnitude of the external magnetic field. Therefore, the performance of the magnetic flux pinning will be directly affected by the size of the external magnetic field, so it is necessary to strengthen the superconductivity of the magnesium diboride, thereby improving the stability of the magnetic flux pinning.

3. Doping study of magnesium diboride

Magnesium boride is a relatively simple alloy. In order to explore higher critical temperatures and higher superconductors, carbon doping is carried out by doping magnesium diboride by using super-cells. Aluminum was doped into magnesium diboride to carry out research.

Since aluminum diboride itself does not have superconductivity, in order to be able to draw data and make comparisons, by listing the structural parameters of aluminum diboride, the specific parameters of the experiment are obtained by optimizing the calculation. The stability parameter value of aluminum diboride, so the structural parameters used in the experiment are all calculated by actual calculation. The nature of metallic aluminum is between metal and non-metal, so the boron-aluminum compound may be an ionic bond or a wage bond. However, it is found through experiments that the formation of chemical bonds between boron and aluminum depends mainly on the distance between boron and aluminum atoms. When the distance between the two is greater than 2.97, the boron atoms and aluminum atoms are ionic bonds. When the distance between them is less than 2.96, the boron atom and the aluminum atom form a wage bond. In simple terms, if the distance between the boron atom and the aluminum atom is long enough, the electron between the boron atom and the aluminum atom will not be shared. If the distance between the boron atom and the aluminum atom becomes very short, then the boron atom The current state of electron cloud overlap is formed between the aluminum atoms. According to the data obtained from many experiments, we can find that when the aluminum diboride is in a sTable state, the distance between the boron atom and the aluminum atom is greater than 2.97, so when the aluminum diboride is in a sTable state, both the boron atom and the aluminum atom are The ionic state naturally forms an ionic bond.

Through a large number of experiments, it is proved that the doping concentration will affect the superconductivity of magnesium diboride. If the doping concentration of magnesium diboride is not large, the superconductivity will be reduced, but it still remains. It is a superconductor, and the nature of the superconductor does not change. When the doping concentration of aluminum in the aluminum diboride reaches a certain high value, the aluminum element will occupy a larger density, which leads to a decrease in the density of boron and magnesium. At this time, the density of aluminum continues to increase, resulting in a composite. The loss of superconductivity, through the study of magnesium diboride, we can easily find that the superconductivity of magnesium diboride is mainly derived from the orbital electrons of boron atoms.

After the carbon element is doped into the magnesium diboride, a 2*2*2 supercell is formed, and the carbon atom replaces the boron atom in the compound. In order to reduce the practice, by utilizing the symmetry of the crystal structure and some approximations In the case of the volume, the dopant is optimized in volume, so that the optimized energy is less than the actual calculated energy, and different data will be calculated in different cases. In the total density of states, the specific gravity of carbon is not very large, and the contribution of the total density of states at the Fermi surface is mainly derived from boron atoms. According to a large number of experimental data, the dopant of magnesium diboride still has weak conductivity when 25% of carbon is doped in magnesium diboride. By comparing the data of magnesium diboride after the addition of the dopant with the data without the addition of dopants, we found that some free electrons that are conductive after the addition of the dopant exist, and when it reaches a certain level, the state of Fermi energy The main influencer of density changes to carbon atoms. At this time, the boron atoms are no longer dominant. Therefore, it is not difficult to find that the concentration of carbon atoms plays a certain degree to change the superconductivity of magnesium diboride.

4. Conclusion

The superconductor magnesium diboride was studied by the linear-enhanced plane wave method (LAPW) using density functional theory (DFT), and from the basic characteristics of magnesium diboride, through the analysis and study of magnesium diboride, The crystal structure and electronic structure of magnesium diboride are also discussed in detail for the conductivity of magnesium diboride. The basic characteristics of the superconductor magnesium diboride are fully described to make the doping of magnesium diboride. The research has become more specific. By using the method of constructing super-cells to study the doping of carbon and aluminum in magnesium diboride, the band structure, density of states and charge density of Fermi surface of magnesium diboride are obtained. And through a large number of experimental data, it is verified that the superconductivity of magnesium diboride is mainly derived from boron atoms, and the four energy bands that can pass through the Fermi surface are boron atoms. Moreover, after super-cell doping of magnesium diboride, the doping carbon atoms and aluminum atomic enabling bands become more saturated than before, thereby achieving the purpose of reducing the superconductivity of magnesium diboride. The experimental data show that some characteristics of doped magnesium diboride superconducting system play an important role in the further study of magnesium diboride doping, and provide a favorable reference for further research on magnesium diboride. The data has opened up a more comprehensive development path for the development of superconducting magnesium diboride and the doping of magnesium diboride.

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