Study on Electronic Structure and Doping of Superconductor Magnesium Diboride

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Abstract: In view of the linear structure of multi-band and dual-band superconducting magnesium diboride, the electronic structure of magnesium diboride is studied by linear structure based on density-based function theory (DFT). The electron doping and hole doping of magnesium diboride were studied by electron band diagram of magnesium diboride and density (DOS) and charge density. The aluminum atom was replaced by aluminum atom and carbon atom. Instead of boron atoms, the change in charge density is derived from which changes are made.

1. Introduction

The superconductor is actually a driver that has no energy loss after power-on. This is mainly due to the large number of pairs of electrons cohering in a coherent state in which crystals are unconstrained and free to diffuse. 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 developed a solution to explore superconductors. People have always dreamed of pursuing room temperature superconductors. 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 cannot 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 this superconductor can still carry ultra-high superconducting current at a temperature of about 20K and at the same time with the earth's magnetic field of 80,000 times, and the energy consumption is extremely low. And it can produce 20K temperature through a small refrigerator, so the scope of application 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 into two. Magnesium borate will greatly reduce the cost of the hospital. Magnesium diboride materials are cheaper and easier to process than high temperature ceramic oxide superconductors, so shortly after they were discovered, an American laboratory stretched and stretched the material out to tens of meters. The superconducting coherence length of magnesium diboride superconductors is longer, so this property can be utilized. Superconducting quantum interference devices have been fabricated to detect electromagnetic signals and promote the development of medical, environmental and military instruments in China.

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 consists of hexagonal Mg atoms, wherein the dense structure is between the B layers of the honeycomb structure, and the graphite space group is P6/mmm. . The lattice parameters obtained by X-ray and structural analysis were a = 3.086 A, c = 3.524 A. Mg and B atoms occupy positions 1a and 2d, respectively, and each element of solid physics contains a formal structural unit (Z = 1).

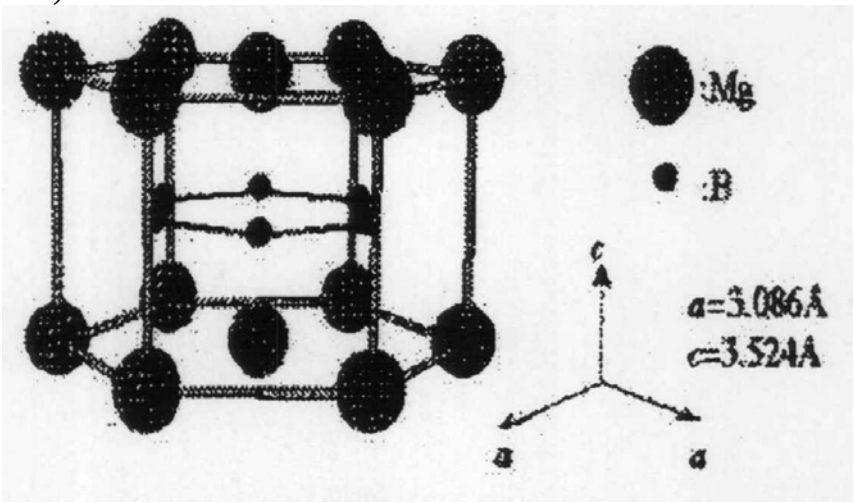

Figure 1 Magnesium diboride crystal structure

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.

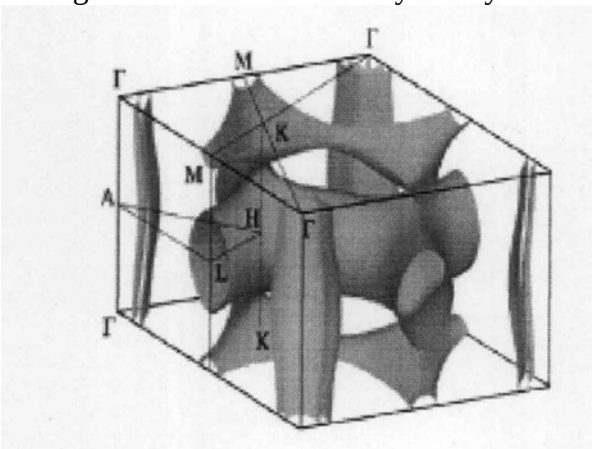

Figure 2 Fermi surface structure of magnesium diboride

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 will decrease with the increase of pressure. By using different methods to verify, we find that phonons play a dominant role. Whether it is high temperature or low temperature, the results are basically the same, and then come along. One problem is that magnesium diboride can continue to carry a large superconducting current when there is a large magnetic field outside. 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 diboride is a structure that is relatively simple alloy, but in order to be able to explore higher critical temperatures and higher superconductors, by doping magnesium diboride, by using super-cells the study was carried out by doping carbon and aluminum into magnesium diboride.

Since aluminum diboride itself is not superconducting, in order to be able to draw data, a comparison is made by listing the structural parameters of aluminum diboride. Through reasonable calculation, we get some specific experimental parameters, mainly the magnesium diboride stability parameter value, then we can explain that the structural parameters used in the experiment are all obtained through actual accounting. Since the metal aluminum is in the properties of metal and nonmetal, it is impossible to specifically judge whether the borosilicate compound makes the ionic bond or the work bond. However, it is found through experiments that the chemical bond between boron and aluminum mainly depends on the distance between the boron atom and the aluminum atom. When the distance between them exceeds 2.97, the boron atom and the aluminum atom generate ionic bonds; when the distance between the two is less than 2.96 the boron atom and the aluminum atom form the 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 phenomenon of electron cloud overlap occurs between the aluminum atoms and the aluminum atoms. According to the data obtained from a large number of experiments, it is not difficult to find that when the aluminum diboride is in a relatively sTable state, the distance between the boron atom and the aluminum atom is greater than 2.97, so the boron atom and the aluminum atom are in a sTable state when the aluminum diboride is in a sTable state. It is an ionic state, which 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, the relative density of carbon is not very large, and the contribution of the total density to 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. The impact.

4. Summary

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 shown that the superconductivity of magnesium diboride is mainly derived from boron atoms, and the four energy bands capable of passing through the surface of the Fermi 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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