First-principles study of anisotropic optical properties of MgB2

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Abstract: By using the first principle of density general function in the study of superconductor MgB2, the anisotropic optical properties of superconductor MgB2 are derived. Through the basic theoretical research on the optical properties and the basic application of the calculation method, the optical spectroscopic and reflectance spectra of MgB2 are derived, and the atomic decomposition state density map of MgB2 is combined with the calculated reflectance spectrum and electron energy loss spectrum. Experimental analysis of each peak is carried out. Through the analysis of the optical spectrum, it is known that there are some differences between the x direction and the z direction in the optical spectrum, but it is not difficult to find the x in the electron energy loss spectrum. The direction is approximately the same as the z direction. From the data reflected from the optical spectrum, the first inter-band absorption peak in the x direction appears at 20000 cm-1, and the first interband absorption peak in the z direction appears at 40,000 cm-1 because of optical properties. Due to the temperature effect, at this time, by adding Lorentz to broaden, and finally through experimental calculation, the experimental results obtained are better than the original data, mainly because the position of the absorption peak between the bands has changed, compared with the previous position. There is a difference of 1000cm-1, but overall, there are no big problems. The overall data reflects the qualitative and quantitative specifics, in the latest error range of anisotropic photoconductive experiments.

1. Introduction

The temperature of the superconductor MgB2 can be as high as 39K, which has been widely concerned by researchers since its discovery, and the research on MgB2 has been paid more and more attention. It was found through research that MgB2 is a simple graphite-like structure, and the formation of MgB2 is produced by inserting a magnesium atom into a boron atom. Using the isotope effect to study MgB2, the phonon mediation of MgB2 can be applied to the BCS theory. The study shows that MgB2 is a metal-type band structure, and the density of Fermi surface states reaches 0.72, thus exploring that MgB2 does not meet the requirements. The research on MgB2 is still going on in a lot, because there are still many problems about MgB2 that need to be solved and it is precisely because MgB2 is a new research superconductor, and the superconductor has improved performance compared with the conventional superconductor, so The great research of MgB2 is the main purpose at present. Therefore, a large number of experiments and researches have confirmed that MgB2 is a double-gap structure, and its energy gap is mainly derived from boron atoms. Different energy gap data are obtained through different experiments, which are mainly divided into 1.5-3.5 meV and 6.0- Within 7.5meV two ranges.

In order to fully study the physical properties of MgB2, we need to use the optical properties of MgB2 to achieve an important method to highlight the physical properties of MgB2. An important experiment to study the structure of solid electrons is achieved by utilizing the action of light probes, which utilizes the interaction between light and electrons to bring the conduction band electrons into a low-energy state. In the analysis of the energy band mechanism of solid electrons, the optical measurement method is used to obtain the specific conditions of the electron band structure, the impurity defect state, and the atomic vibration while the solid light is absorbed. Due to the reflectivity of the light, there is a partial light reflection phenomenon when the light is illuminated by the solid. Moreover, after the light enters the solid, part of the light is absorbed, so that the intensity of the light is affected by the depth of the light entering the solid, and the intensity of the

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light is proportional to the depth of the light incident on the solid.

The structure of the MgB2 crystal is a hexagonal close-packed structure, and since the lengths of the c-axis and the a-axis are very similar, it is difficult to form an oriented MgB2 single crystal. Therefore, the single crystal used for the supply experiment is very scarce, and the long-term study on the optical properties of MgB2 cannot be carried out smoothly, resulting in the incomplete research on MgB2. The study of the optical properties of MgB2 seriously lags behind the research on other aspects of MgB2. With the rapid improvement of the level of computer technology, the study of basic physical properties can calculate the obvious advantages of certain physical properties through the electronic structure of the basic density function theory. A lot of calculated data can promote the progress of the experiment, and open a clear channel for the experiment from the basic data. In order to understand the nature of MgB2, we found the best conditions for this experiment through experiments, and we calculated the optical properties of MgB2 by using the first-principles comprehensive analysis, and obtained the photo-spectrum, and Data such as electron energy loss spectra. Through the calculation of the data results for multiple data comparison, and finally by comparison with the experimental data, we compare, the experimental data and the calculated data are slightly different, that is because of this weak difference, it is likely This leads to data errors and errors in the direction of the research, so preliminary analysis shows that the main cause of this weak difference lies in the error of the calculation system. Through the study of the anisotropic optical properties of MgB2, we obtained more comprehensive data, and these data were confirmed in other large experiments.

2. Optical properties of MgB2

In order to understand the electronic structure of MgB2, understanding of the optical structure of MgB2 can be achieved through the study of optical properties. The interaction between light and electricity can make the conduction band electrons in a low energy form, and can understand from the experimental measurement data. Go to the electronic band structure and then get the electronic band structure, so that you can get more information about the electronic mechanism. Since the dielectric function is an important physical quantity of the microscopic physical process of electronic structures and electronic transitions, it can effectively feedback the energy band structure and related spectral information of the solid. If the effect of absorption is to be considered when light propagates through the crystal, the dielectric function needs to be represented by a complex number.

When light propagates through a medium, it is always affected by the medium, which affects the intensity of the light. Usually, we use the relationship between the refractive index and the dielectric constant to obtain the relevant data, and the calculated data is used. Statistics show the broken line statistics (Figure 1), which shows that the refractive index and extinction coefficient of MgB2 change with the change of photon energy. By comparing with the MgB2 dielectric function curve of Figure 2, we can easily see the relationship between the two.

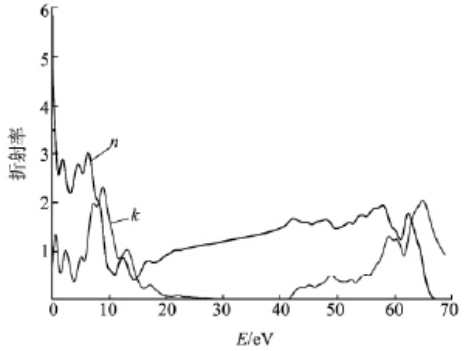

Figure 1 Refractive index of MgB2

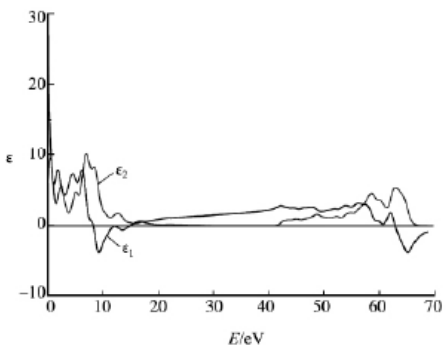

Figure 2 The dielectric function of MgB2

If the light is directly irradiated into the medium of negative refractive index, the amplitude ratio of the reflected wave to the incident wave will change with time, we can get the relationship

between the two, so that the reflection coefficient of MgB2 is obtained by calculation. The change of photon energy, the reflection coefficient is not always in a changing state, he changes irregularly with the size of the photon energy. When the frequency reaches a certain height, the light will not propagate in the crystal, so we need to experiment with the range that the crystal can withstand. The ratio of the unit distance of light propagation in the medium to the light intensity is the absorption coefficient. Due to the existence of the extinction coefficient, the light cannot be completely transmitted, so the absorption coefficient in the medium is proportional to the extinction coefficient.

3. Calculation method

The A1B2 type is a crystal structure of MgB2, and is formed by inserting hexagonal close-packed Mg atoms into the carbon element B layer. Therefore, the Mg atom and the B atom together constitute MgB2. The spatial symmetry group of its crystal structure is P6/mmm. In this paper, the electron band structure is studied by analyzing the energy band structure and by using the scheme of the full potential line model track, and the dynamic matrix is calculated by using the linear response method, and then the electroacoustic is calculated. The combination of sub-interacting matrices gives better feedback data. By using the lattice wave function to calculate the relevant data about Mg in B, and the data acquisition for MgB2 is technically required by one point, combined with the generalized gradient approximation method, the electronic part and the phonon part can be calculated. In order to study the method of calculating MgB2, this is the tetrahedral method. When calculating the 28 wave vectors that can be used in the Brillouin zone, the Brillouin zone is divided by the same method, so that the data is more comprehensive and reliable. The influence of the band structure and the Fermi surface can bring more accurate data reference for linear response calculation. Therefore, the role of MgB2 and the value of data utilization are more concretely expressed.

4. The calculation results

The electron band structure and density of states before and after stretching of the MgB2 film were calculated to obtain the case of Fig. 3. The lattice constant before stretching was a = 0.3196 nm, c = 0.3612 nm; the lattice constant after stretching was a = 0.3125 nm, and c = 0.3621 nm. The solid line in Fig. 3(a) indicates the electron energy band before stretching, and the dotted line indicates the electron energy band after stretching. The solid line in Fig. 3(b) indicates the total density of states before stretching, the broken line indicates the density of the p-state partial states of B before stretching, and the dotted line indicates the total density of states after stretching and the density of states of p-state of B. Through the feedback in the figure, it is not difficult to understand that in Fig. 3, the superconductivity of MgB2 is mainly due to the α-band of B. By showing the planarity, the density of states around the Fermi surface shows Van Hoff. According to the comparison of the data in the Table, the lattice constant of MgB2 film has not changed greatly, and the density of states of electron band and Fermi surface has not changed greatly. The main reason is that the p electron of B plays a role. After the plane stretching of the MgB2 film, the lattice constant is continuously increased, resulting in a decrease in the density of states. However, by analyzing the state partial density and total density of the state before and after stretching, the data about MgB2 is obtained, and the situation reflected from the data is not greatly changed.

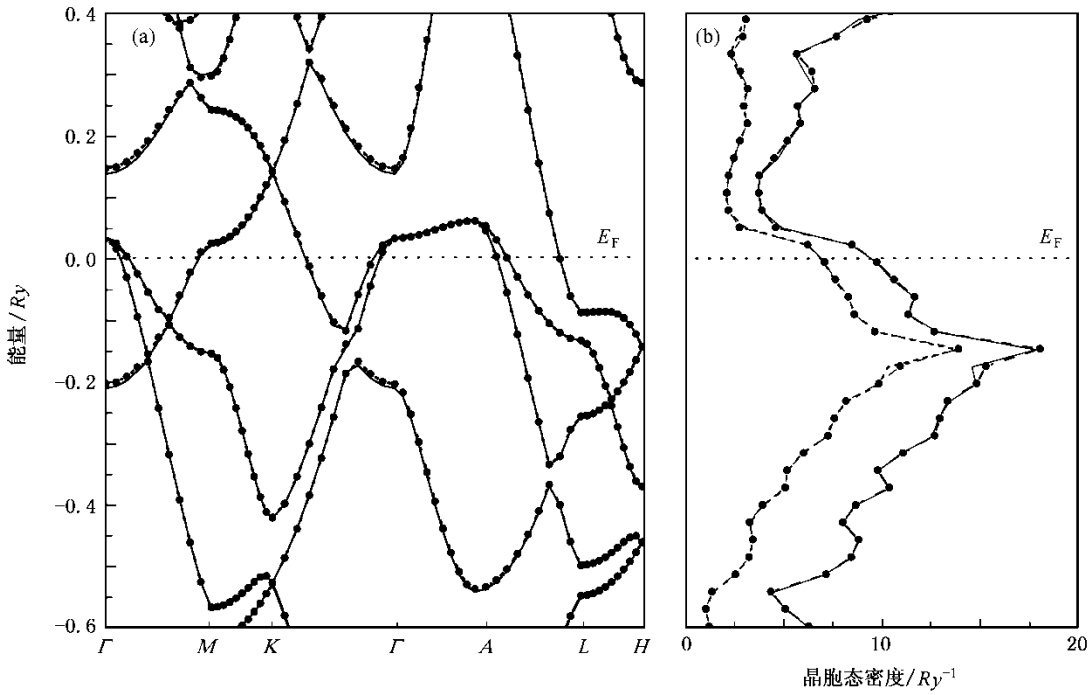

Fig. 3 Electron band structure and density of states before and after stretching of MgB2 film (a) Electronic band structure, the solid line in the figure indicates the electron band before stretching, the dotted line indicates the electron band after stretching; (b) Density, the solid line in the figure indicates the total density before and after stretching, the dotted line indicates the density of the p-state partial state of B before and after stretching, and the dotted line indicates the total density of states after stretching and the density of p-state partial states of B.

5. Conclusion

In this paper, the optical properties of MgB2, such as photo-spectrum, reflection spectrum and electron energy loss spectrum, are studied by using the first-principle of density-reverse function. The results are the same as the experimental data, which leads to a more detailed description of MgB2. research data. Through the use of modern computer science methods, the various parameters obtained have opened up a smooth channel for the study of the optical properties of MgB2, which has played a key role in the research results and optical properties of MgB2.

References

[1] Shang Xuefu, Tao Xiangming, Chen Wenbin, Chen Huixian, Wang Wei, Tan Mingqiu. First-principles study of anisotropic optical properties of MgB_2 [J]. Acta Phys. Sin., 2008(09): 5838-5843.

[2] Wu Yong. First-principles study on the electronic structure and bonding properties of a novel superconductor MgB_2 [J]. Journal of Capital Normal University (Natural Science Edition), 2002(01): 23-27.

[3] Zhi Xiaofen. First-principles study of electronic structure and optical properties of MgB_2 doping system [D]. Qufu Normal University, 2009.

[4] Shu Huabing, Liu Su, Ma Rong, Liu Wei. First-principles calculation of the effect of stretching of MgB_2 film on superconductivity [J]. Acta Phys. Sin., 2007(12):7262-7265.