Theoretical Calculation of Electronic Structure and Optical Properties of MgB2

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Abstract: This paper uses the first principle of Density functional theory (DFT) to theoretically calculate the electronic structure parameters and optical properties of MgB_2 superconductors. In the analysis of electronic structural parameters, the unitary model of MgB_2 was optimized by generalized gradient approximation and local density functional approximation, and the lattice parameters of the model were adjusted. The dielectric constant spectrum of photon energy and MgB_2, the refractive index of MgB_2, the photon reflection spectrum, the photon absorption spectrum and the energy loss function of MgB_2 were obtained by calculation. Through the comparison of various relational graphs of MgB_2, the conclusion that they have a mathematically proportional correspondence is obtained.

1. Introduction

MgB_2 is a superconductor material with a wide range of raw materials, low price, simple chemical structure and easy synthesis and processing. It is also a key material for research and development in many fields such as superconducting force transmission and micro-nanoelectronic devices. Although MgB_2 is a simple crystal, single crystal Growth is difficult, and actual research progress is getting slower. In this paper, the theoretical calculation of the electronic structure and optical properties of MgB_2 from the perspective of DFT is carried out, and the calculated results are compared with the state density of MgB_2 and the energy loss function to verify the accuracy of the calculation results.

2. Rational model and its calculation method

In this paper, density functional theory (abbreviation: DFT) is used for calculation. In DFT, the Schrödinger equation for a single electron motion can be expressed by equation (1).

$$\left[-\frac{\dot{y}^2}{2}-\sum_q\frac{Z_q}{|r-R_q|}+\int\frac{\rho(r)}{|r-R_q|}dr+V_{xc}\right]\times\psi_i(r)=\varepsilon_i\psi_i(r) \quad (1)$$

$$,\rho(r)=\sum_i n_i|\psi_i(r)|^2 \quad (2)$$

In the formula (1), $\psi_i(r)$ represents a single electron wave function of MgB_2, $n_i$represents the eigenstate electron occupancy of MgB_2, and$\rho(r)$ represents the multielectron density of MgB_2. In the formula (1), the $\frac{\dot{y}^2}{2}$term represents the effective electron kinetic energy of MgB_2 in the system; the $\sum_q\frac{Z_q}{|r-R_q|}$term is the Coulomb attraction potential of each atomic pair of electrons, expressed by a regular pseudopotential; $\int\frac{\rho(r)}{|r-R_q|}dr$ is the Coulomb potential; $V_{xc}$is the exchange-related potential expressed by the approximation method.

In this paper, the PBE density functional in generalized gradient approximation is used to determine the exchange potential of MgB_2, and the correlation energy of MgB_2 is determined by the CA-PZ functional in the local density functional approximation. In the actual calculation, the cell of the multi-body MgB_2 system is subdivided into network nodes initialized with the$\psi_i(r)$probe wave function, and then the network node for solving the eigenequation (1) is calculated according to equation (2). The Kohn-Sham potential. The solution of the eigenfunction

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$\psi_i(r)$is often different from the value of the initialized$\psi_i(r)$, so a part of the newly solved wave function needs to be added to the value of the initialized $\psi_i(r)$, and the modified Kohn is iteratively calculated. -Sham potential (2), repeat the above steps until the value of $\psi_i(r)$converges to a sTable number, the value of which is the value of the single electron wave function$\psi_i(r)$ representing the total energy of the system and the density distribution of the charge.

In this paper, the calculation accuracy of the regular pseudopotential calculation of atomic electrons in the reciprocal space of the crystal is 1×10^{-6}Ev/atom Ev/atom, and the orbits related to MgB_2 are $Mg(3s^2)$and $B(2s^2 2p^1)$. In the k-space of reciprocity, the k vector is selected as 9×9×8, and the ground state energy of Mg and B valence electrons is iteratively calculated. The final calculation result is Mg-22.891eV, B-70.912eV, and the plane wave cutoff energy is 400.00eV. In the Brillouin area, the charge density and the total energy of the system are calculated. The ground state energy is selected by the density mixing algorithm. The convergence accuracy of the Fermi energy is 7.50×10^{-8}eV, and the convergence accuracy of the electron energy eigenvalue is obtained. At 7.50×10^{-7}eV, the convergence accuracy of the bandgap is 1.00×10^{-5}eV The force requirement on each atom is lower than 1.0×10^{-1}eV/nm, the stress deviation is less than 2×10^{-2}Gpa,, the tolerance offset is less than5.0×10^{-3}nm

In this paper, the hexagonal structure model of MgB_2 crystal is used for calculation. The space group P6/mmm international code 191, hexagonal close-packed structure, its structural calculation model is shown in Figure 1, magnesium atom occupies 1a(0,O,O,)Boron atoms occupy 2d (1/3, 2/3, 1/2) positions, each containing a magnesium nucleus and two boron atoms. The initial lattice parameter is set to $a = 3.086 \times 10^{-10}$m, $c = 3.524 \times 10^{-10}$m, and the optimized lattice parameters are adjusted to $a = 3.057 \times 10^{-10}$m, $c = 3.519 \times 10^{-10}$m.

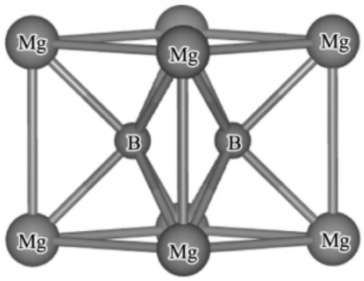


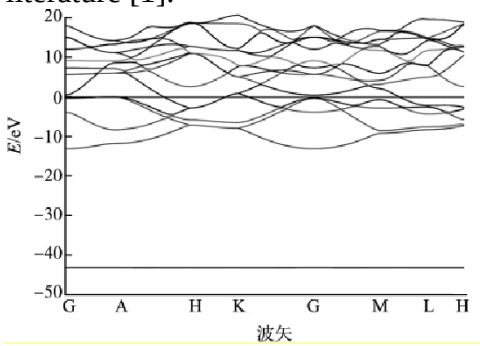
Figure 1 MgB_2 crystal unit cell structure

3. Calculation results and data analysis

3.1 Electronic structure analysis of MgB_2 superconducting crystal

Figure 2 is an energy band structure diagram based on generalized gradient approximation and local density functional approximation. Figure 3 is the total density of states of MgB_2. It can be seen from the figure that the density of states of MgB_2 is corresponding to the band structure diagram. The fluctuations of -15eV~23eV and -43eV are highly correlated. Moreover, in the calculation result, the Fermi level E_F=0 is near, and the density density curve of MgB_2has a concave gap E_g. The appearance of the left peak of the gap is caused by the bonding state of Mg-p and Bp hybridization, while the peak of the right side of the gap is due to the reverse bond formed by the hybridization of Mg-p and Bp. It can also be seen in the analysis of the atomic density of each atom. From the disguise density map, the chemical bond bonding of Mg and B atoms can be analyzed and the weight contribution to the density of states can be found. Figure 4 is a graph showing the density of the Mg atoms and B atoms. It can be seen from the figure that the filling of 2p electrons of Mg results in an electronic state of -44.162 to -42.259 eV, and the hybridization of s and p electrons of Mg atoms and B atoms. The conduction band and the valence band between -14.040 and 24.195 eV are overlapped. The formation of the conduction band is mainly due to the 3s and 3p orbitals of Mg atoms in MgB_2, partly because of the 2p and 2s orbitals of B atoms; the formation of valence bands is facilitated by the 2s orbitals of B atoms and 2p orbitals, and there are

almost no Mg 3s and 3p orbitals. Contribution. For the bonding properties of MgB_2, reference can be made to the literature [1].



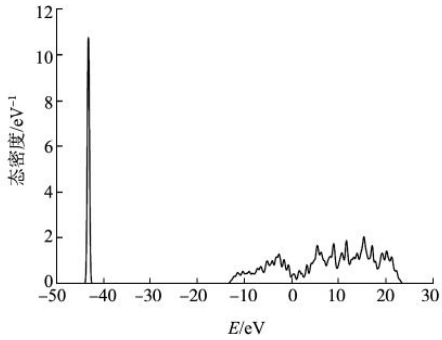


Fig. 2 Analysis of the energy band structure of MgB_2 Figure 3 Density analysis of MgB_2

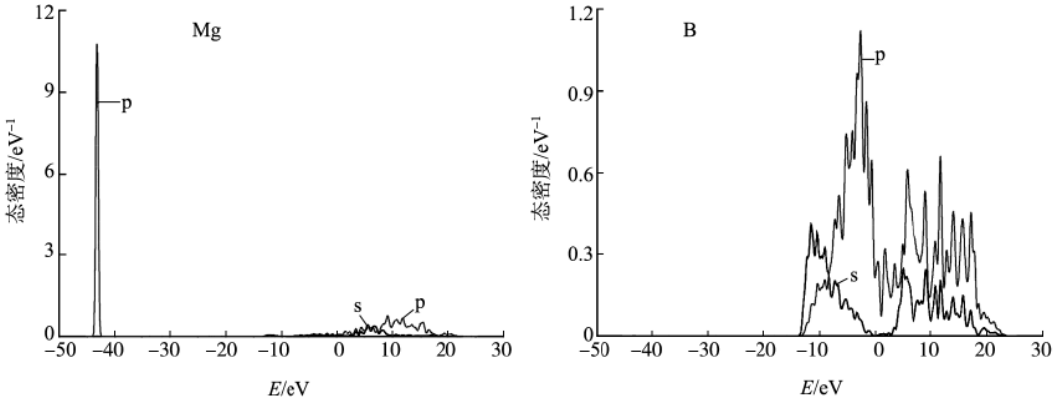
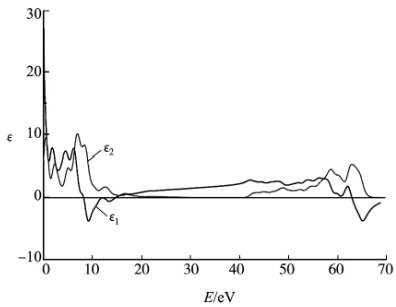


Fig. 4 Analysis of the density of MgB_2

3.2 Optical properties

The dielectric function is a function image obtained by optical experiments to obtain the photoelectric interaction relationship of materials. It is often used to derive the electronic structure information of the energy band structure of the material. In this paper, the dielectric constant of light in MgB_2 medium is ε(ω)=ε_1. +iε_2 (ω) indicates.

By calculation, the refractive index, reflectance, dielectric constant spectrum, energy loss function and absorption spectrum of MgB_2 were obtained. Figure 5 is a graph of the real part Re(ε) = ε_1 and the imaginary part Im(ε) = ε_2 of the MgB_2 dielectric constant as a function of photon energy. As can be seen from Fig. 5, when the photon energy is lower than 6.5 eV, ε_1 is relatively large; when the photon energy is 8.230 to 14.868 eV and 62.914 to 68.761 eV, light cannot propagate in the crystal because ε_1 is less than 0 at this time. The calculated static dielectric constant $\varepsilon_1(0) = 29.821, \varepsilon_2(0) = 6.079$.



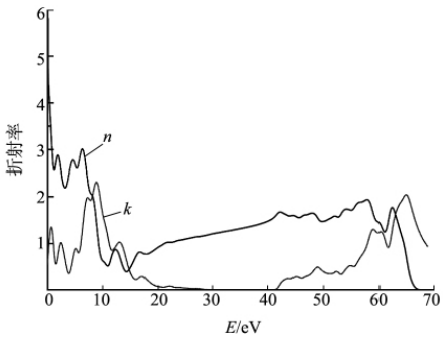


Fig. 5 Dielectric constant spectrum of MgB_2 Figure 6 refractive index of MgB_2

The speed of light propagation in the medium is equal to the speed of the vacuum light divided by the refractive index, ie $v = \frac{c}{n}$, where $n = \sqrt{\varepsilon}$. The refractive index n in the absorption medium should be represented by n = i + k in the complex domain. There is a function relationship between

$(n+ik)^2=\varepsilon$ between the refractive index and the dielectric constant, and it is easy to derive $\varepsilon_1=\varepsilon^2-k^2$, $\varepsilon_2=2nk$. Fig. 6 is a graph showing the relationship between the extinction coefficient k and the calculated refractive index n as a function of photon energy. The calculation results in $n_0=5.490$. Comparing Figure 6 with Figure 5, it is not difficult to see that there is a certain correspondence.

When the light is vertically injected into the medium with a negative refractive index, the amplitude of the reflected wave and the incident wave will be shifted. The amplitude ratio is $\frac{E_{反}}{E_{入}}=\frac{n-1-ik}{n+1+ik}$, its reflection coefficient is $R=\left|\frac{E_{反}}{E_{入}}\right|^2=\frac{[(n-1)^2+k^2]}{[(n+1)^2+k^2]}$, Fig. 7 is a calculated MgB_2reflection spectrum reflecting the relationship between the reflection coefficient and the photon energy. As can be seen from the figure, when the photon energy reaches 9.640 eV, it corresponds to the energy when $\varepsilon_1(\omega)$ first obtains a negative maximum value, and the reflection coefficient is large at this time. When the photon energy is greater than 63.000 eV, the reflection coefficient increases rapidly, and the propagation of light at this frequency in the crystal is limited, which also corresponds to the energy range when $\varepsilon_1(\omega)$ takes a negative value for the second time.

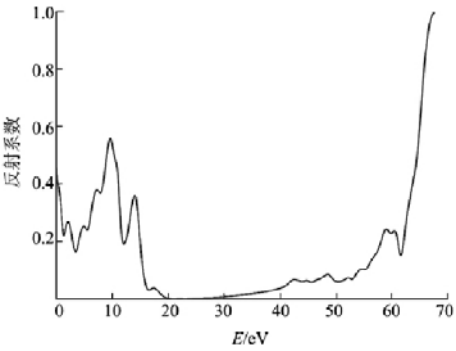


Figure 7 Photon reflection spectrum of MgB_2

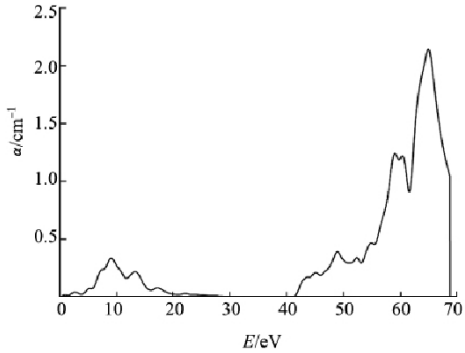


Figure 8 Photon absorption spectrum of MgB_2

The absorption coefficient of light in the medium MgB_2 is attenuated by $e^{-\frac{2\omega kx}{c}}$, and its absorption coefficient$\alpha=\frac{2\omega k}{c}=\frac{4\pi k}{\lambda_0}$. The absorption coefficient α is proportional to the extinction coefficient k. Fig. 8 is a graph showing the relationship between the absorption coefficient of MgB_2 and the change in photon energy. As can be seen from the figure, the absorption coefficient is almost zero at 33.1 to 41.2 eV, and the absorption peak is at 64.098 eV, and the absorption coefficient at this time is$\alpha=2141879.216\text{cm}^{-1}$. By comparison, it can be found that the absorption coefficient in Fig. 8 is similar to the extinction coefficient curve in Fig. 6, because there is a relationship of$\alpha=\frac{4\pi k}{\lambda_0}$ between them.

The energy loss function, $L(\omega)=-\text{Im}\left(\frac{1}{\varepsilon}\right)=\frac{\varepsilon_2}{(\varepsilon_1^2+\varepsilon_2^2)}$, is used to describe the energy loss of charged particles as they pass through a solid. In theory, it is usually The reciprocal of the negative dielectric constant is defined as the energy loss function. Figure 9 is a graph of the calculated electron energy loss function versus photon energy change. The peak of the loss function is important data to characterize the plasma oscillation, and its corresponding frequency corresponds to the oscillation frequency of the plasma. As can be seen from the figure, the peak value of the energy loss function is also around 15.25 eV, and the value is 2.49, which corresponds to the reflection spectrum of Fig. 7, and a conclusion similar to the reflection spectrum is obtained.

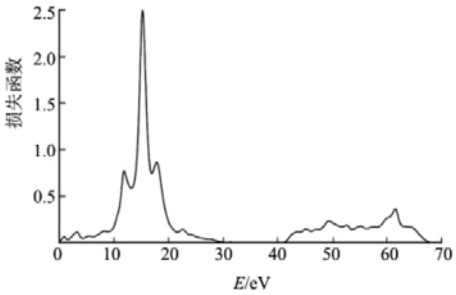


Figure 9 Energy loss function of MgB_2

4. Conclusion

Based on the first principle of DFT, this paper uses local density functional approximation and generalized gradient approximation to approximate, optimizes the geometry of MgB_2 model, and calculates and discusses the electronic structure parameters. The obtained lattice parameters are obtained. It is in good agreement with the experiment; for the optical properties of MgB_2, the refractive index, photon absorption spectrum, photon reflection spectrum, dielectric constant spectrum and energy loss function of MgB_2 are calculated respectively, and the static dielectric constant of MgB_2 is obtained $\varepsilon_1 = 29.821$, $\varepsilon_2 = 6.079$, $n_0 = 5.490$, the peak value of the energy loss function is 2.49, and the peak value of the absorption coefficient$\alpha = 2141879.216\text{cm}^{-1}$.

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