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Electronic structure of MgB_2

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Abstract. Results of *ab initio* electronic structure calculations on the compound MgB_2 using the FPLAPW method employing GGA for the exchange-correlation energy are presented. Total energy minimization enables us to estimate the equilibrium volume, c/a ratio and the bulk modulus, all of which are in excellent agreement with experiment. We obtain the mass enhancement parameter by using our calculated $D(E_F)$ and the experimental specific heat data. The T_c is found to be 24.7 K.

Keywords. Electronic band structure; superconductivity.

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1. Introduction

The discovery of superconductivity in MgB_2 (T_c 39 K) by Akimitsu [1], has led to a great deal of interest in this compound. At ambient conditions it crystallizes [1] in the layered hexagonal AlB_2-type structure. Boron isotope effect [2] has been observed in MgB_2 revealing that the pairing mechanism leading to superconductivity is of phononic origin. The electronic band structure combined with strong coupling superconductivity theory can therefore be expected to give a good quantitative description of this compound. Motivated by this, we have carried out *ab initio* electronic structure calculations using the full potential linear augmented plane wave method (FPLAPW) employing the generalized gradient approximation (GGA) for the exchange-correlation energy. We used the McMillan formula [3] to estimate T_c. Here we briefly describe our method and calculations, and present our results and conclusions.

2. Electronic structure calculations

We have performed *ab initio* electronic structure calculations using FPLAPW as implemented in the WIEN97 code [4]. The basis functions are the radial solutions of the Kohn–Sham equation inside the atomic spheres. We use plane waves in the interstitial region. The solution inside the atomic sphere includes spherical and non-spherical components of the potential. The exchange-correlation terms have been treated within the GGA. We calculate and minimize the total energy with respect to the c/a ratio as well as the volume. Here a and c are the lattice parameters of MgB_2 which crystallizes in hcp (AlB_2) structure. We

have determined the total energy as a function of volume whose derivative we take to get the bulk modulus B. We obtain the total density of states at the Fermi level $D(E_F)$ from our calculated band structure to determine the electronic specific heat coefficient γ. Comparing it with the experimental γ_{exp} [2] we estimate the mass enhancement factor which is then used to determine the electron–phonon coupling constant λ. Choosing suitable values for the Coulomb pseudopotential μ^* and the Debye frequency ω_D we finally obtain T_c.

3. Results and discussion

Our calculated c/a ratio is 1.1510 and equilibrium volume V_0 is 194.0785 Å. These numbers compare well with the experimental values [1] of $c/a = 1.142$ and $V_0 = 196.0388$ Å. Our calculated bulk modulus is $B = 148$ GPa compared to the experimental value [5] of $B_{exp} = 152$ GPa. We show in figure 1 the calculated band structure. Notice that at the Fermi energy there is a flat band which is predominantly of boron 2p origin. This band makes a large contribution to the density of states at the Fermi energy $D(E_F)$. We show in figure 2 the electron density distribution in the plane containing the Mg atoms and in figure 3 for the plane containing both Mg and B atoms. It is seen from the density distribution of figure 2 that the electronic transport in this plane would be metallic. In figure 3 we see a different situation where the high electron density between the B atoms is an indication of covalent bonding. The experimental estimate of γ is $\gamma = 3 \pm 1$ mJ/mol$-K^2$ whereas our calculated γ is 1.7 mJ/mol$-K^2$. Using the relationship $\gamma_{exp} = (1 + \lambda)\gamma$ we find that the dimensionless electron–phonon coupling constant $\lambda = 0.765$. Choosing the values $\mu^* = 0.11$ [6] and $\omega_D = 750 \pm 30$ K [2] we obtain T_c using the McMillan formula:

$$T_c = \frac{\omega_D}{2.4} \exp \frac{-1.04(1+\lambda)}{\lambda - \mu^*(1 + 0.62\lambda)}.$$

This yields a $T_c = 24.7$ K. We thus find that a phonon mediated theory of strong coupling superconductivity gives a reasonable value of T_c. The large value of λ indicates strong

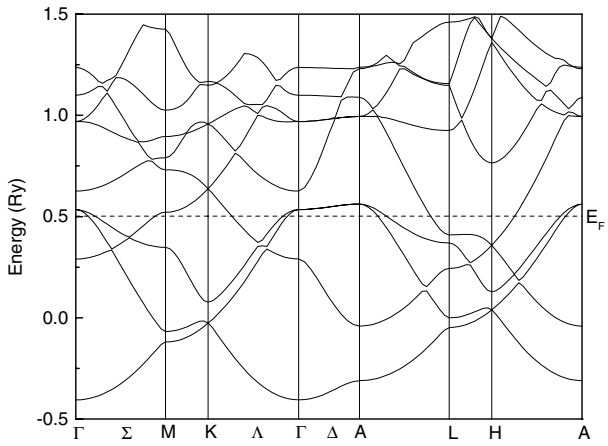

Figure 1. Band structure of MgB_2 along different symmetry directions.

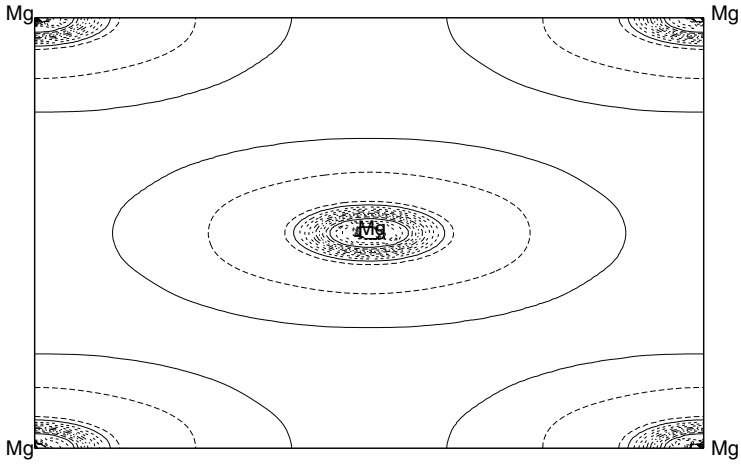

Figure 2. Electron charge density distribution in the (110) plane of the hcp structure. The units along X and Y axes are arbitrary.

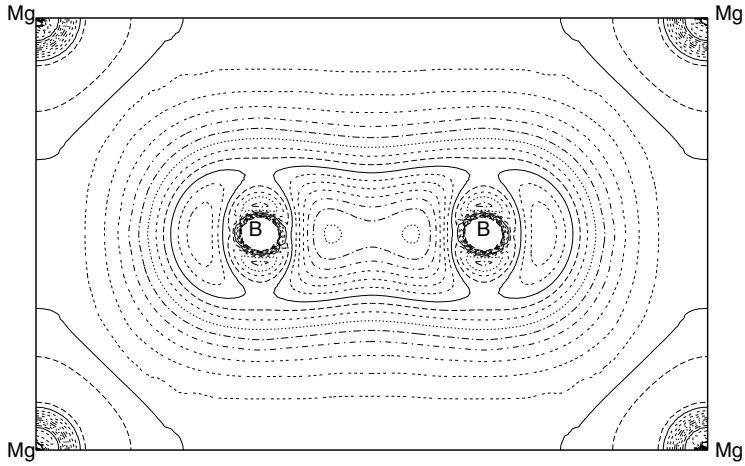

Figure 3. Electron charge density distribution in the (100) plane of the hcp structure. The units along X and Y axes are arbitrary.

coupling superconductivity. The high transition temperature is largely due to the large density-of-states at the Fermi energy coming from the B 2p band. It will be interesting to see the effect of pressure on this band and its consequent effect on T_c which will provide an important clue to explain its experimental variation with pressure.

Note: After the completion of this work, we learnt of the work by Kortus *et al* [7] who have obtained results similar to ours.

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