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Comparative study of the electronic structure of alkaline-earth borides (MeB_2; Me = Mg, Al, Zr, Nb, and Ta) and their normal-state conductivity

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Abstract

By means of density functional theory the electronic structure of the MgB_2 superconductor was characterized and compared with that of the related iso-structural systems: AlB_2, ZrB_2, NbB_2, and TaB_2. Using the full potential-linearized augmented plane wave (FP-LAPW) method and the generalized gradient approximation, the electronic density distribution, density of states, and band structures were obtained for these compounds. The electrical conductivity, which cannot be easily measured in the *c*-direction, was calculated, in the relaxation time approximation using band structure results. It was found that the two-dimensional (2D) crystal structure character of these metallic diborides is also reflected in the electronic charge distribution. This 2D pattern is not reproduced in the electrical conductivity as it is, for instance, in the superconductor high T_c cuprates. The calculations indicate a bulk, yet anisotropic, conductivity for all these compounds.

1. Introduction

Since a superconductive transition was reported in MgB_2 [1], a considerable effort has been made in order to understand the origin of such an electronic phase transition for this kind of intermetallic compounds. In this regard, several other compounds with the boron-layered crystal structure have been studied [2–4]. The subjacent idea was to keep the two-dimensional (2D) boron crystal substructure, where superconductivity is supposed to occur and to modify the magnesium layer by alloying with other metals in order to understand the phenomenon as well as to optimize the superconductivity in this intermetallic compound. Taking into account all the potential applications of MgB_2, studies of the anisotropic properties of this type of materials are of considerable importance for a fundamental understanding of the associated superconductive and normal states. It is well known that anisotropy strongly affects the flux pinning and critical currents. These parameters have to be considered for the design of novel electronic devices. Therefore, MgB_2 could be one of the best candidates to replace the Nb-based materials in applications of superconductivity.

In summary, the physical and chemical properties exhibited by the metallic diborides, MgB_2 and related compounds made them one of the most promising materials for technological applications of superconductivity. The characterization and understanding of these compounds could lead to the design of systems that offer better critical superconducting parameters than the Nb-based alloys and the high T_c cuprates.

Within the framework of the theory of superconductivity, the discovery of superconducting properties in MgB_2, $T_c \sim 40$ K, has motivated a wide reconsideration of the physical parameters that influence the value of the critical temperature in such intermetallic system. Among some earlier explanations were those that considered the importance of the strength of the electron–phonon coupling constant. For MgB_2, Yildirim et al. proposed that a possible mechanism can be due to a strong and

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non-linear electron–phonon coupling resulting from the in-plane anharmonic boron phonons [5]. Another possibility could be associated to the 2D character of the Fermi surface [6,7]. That is, a 2D or anisotropic character was suggested for the superconductivity of MgB_2.

Even though there exist a consensus with respect to the BCS-based explanation of the superconductivity phenomenon in MgB_2, being a fairly typical intermetallic electron–phonon-mediated BCS superconductor, there are several aspects exhibited by MgB_2 that are more closely related to that of high-T_c cuprates (except for the infinite-layer cuprates). For instance, MgB_2, appears to show (a) holes as charge carriers in conductivity, as evidenced from theoretical considerations and Hall effect measurements [8,9] and (b) a low density of states at the Fermi level, something not expected for a conventional superconductor with such a high T_c. From a structural point of view the layered structure of these borides resembles, to some extent, the kind of layer arrangement exhibited by the infinite-layer structure of the superconducting cuprates. The recent discovery of superconductivity [10] at 14 K in $CaSi_2$, another AlB_2-type structure compound, suggests that this structure type may be favorable for superconductivity.

Taking into account that MgB_2 consists of alternating B and Mg sheets, anisotropic electronic properties could be anticipated, resulting from a different in-plane and inter-plane bond character. Similar to graphite, MgB_2 with different B–B in-plane and inter-plane distances should exhibit a strong anisotropy in its thermal, mechanic and electronic properties. Electronic structure calculations have shown that the inter-plane Mg–B bonding is weak compared to the in-plane bonds that have σ-character derived from the B :$p_x + p_y$ electrons (this was also found by Ravindran et al. [11]). The in-plane boron bonds are covalent, while the inter-plane Mg–B bond is strongly ionic.

An important question is how strongly the MgB_2 layered structure is reflected in the electronic properties of MgB_2 and the anisotropic character of its properties. Single crystals are difficult to make and very thin [12–14], making c-direction electrical conductivity measurements almost impossible; therefore, theoretical predictions should be of great value. High-resolution X-ray powder diffraction showed that under high pressure up to 8 GPa, the cell parameter ratio, c/a, is essentially constant [15]; indicating a three-dimensional (3D) character of the mechanical properties of MgB_2. The same conclusion was achieved by Prassides et al. [16] indicating that MgB_2 is a stiff tightly packed incompressible solid with only moderate bonding anisotropy between inter- and intra-layer directions. On the other hand, in a lower pressure experiment (up to 0.62 GPa) it was found (by neutron diffraction) that this system exhibits a unusual large anisotropy in thermal expansion and compressibility [17]. This work also reports that the thermal expansion ($200\,K \leqslant T \leqslant 300\,K$) along the c-axis is twice that along the a-axis; compression along the c-axis is 64% larger than along the a-axis. These last results look consistent with the expected anisotropy arising from the large difference in bond strengths. The B–B bonds in the basal plane being much stronger than the B–Mg bonds that connect layers of B and Mg atoms.

In the superconducting state MgB_2 single-crystal measurements have shown an upper critical field anisotropy (defined as $\gamma = H_{c2}^{ab}/H_{c2}^{c}$) ratio ranging from 1.7 to 2.7 [12–14]. The different values can be attributed to a different quality of the single crystals leading to normal-state magnetoresistive effects. On the other hand, the field-induced resistive transition measurements in MgB_2 [18] have revealed that there is no-significant difference in T_c for the two magnetic field orientations.

2. Computational procedure

The calculations were done using the *WIEN97* code [19], which is a full potential-linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT). The generalized gradient approximation of Perdew et al. [20] was used for the treatment of the exchange-correlation interactions. The energy threshold to separate localized and non-localized electronic states was -6 Ry. For the number of plane waves the used criterion was R_{MT} (Muffin–Tin radius) $\times K_{max}$ (for the plane waves) $= 9$; except for TaB_2, where $R_{MT} \times K_{max} = 8$. The number of k-points used was 6000 (320 in the irreducible wedge of the Brillouin zone). The assigned Muffin–Tin radius for the *Me* atoms was chosen constant for the different compounds and equal to $1.8a_0$ (a_0 is the Bohr radius). This criterion fulfilled the computational requirements of the program and was done so that the calculated properties, density of states (DOS), charge, etc. could be compared consistently. For the boron atom, R_{MT} was equal to half of the B–B internuclear distance. For the convergence the charge density criterion was used, with a value of 10^{-4}. For the charge density plots the semicore states were included ($e_{min} = -9$ Ry).

3. Crystal structure

The crystal structure of MeB_2 (*Me* = Mg, Al, Zr, Nb, and Ta) belongs to the $P6/mmm$ group (191) with *Me* in site a and B in site d. This structure is extraordinarily simple in comparison to that of the high T_c superconductors. The boron atoms lie in planes with a honeycomb arrangement (like graphite), and between two contiguous planes there are the *Me* atoms on the line passing through the center of the boron hexagons.

This structural feature is comparable to that of the infinite-layer high T_c cuprates, on which there are CuO_2 planes with the rare earth atoms lying between the CuO_2 layers, on a line passing through the center of the squares. It is well known that in the high-T_c cuprates, the superconductivity is carried out along the CuO_2 planes, that is, the 2D structural character is reflected in the electronic and conductivity properties.

As the MeB_2 crystal structure also has a strong 2D arrangement, it is an interesting question if this 2D character is reflected in its electronic properties. The objective of this research is the study of the extent to which this 2D geometry is reflected or imposed on the electronic structure and in the anisotropy of the electrical conductivity. The analysis will be done in terms of the calculated charge density, band structure, and density of states as well as on the nature of the chemical bonds. As will be shown below, the 2D character in the electronic properties of these compounds seems to be enhanced by the ionic character of the $Me-B$ bonds.

The cell dimensions were taken from experimental values reported in the literature [1,21,3]. These were (Me, a(Å)/c(Å)): Mg, 3.0864/3.5215, Al, 3.005/3.252, Zr, 3.17/3.532, Nb, 3.111/3.267 and Ta, 3.087/3.247.

4. Results and discussion

4.1. Charge density

4.1.1. MgB_2

The charge density profiles for MgB_2 are shown in Fig. 1 for two planes, and in Fig. 2 for two different crystal paths. These profiles reveal that, in the boron plane, the B–B covalent bond holds a considerable amount of charge, while at the center of the boron hexagons the charge drops to quite a low value, at about 1/8 of the value at the B–B bonds. On the other hand, the magnesium plane exhibits a flat density between the Mg atoms, with the same small value than that found at the center of the boron hexagons (see Fig. 2). Nevertheless, near the magnesium atoms the charge density increases sharply, as expected. These results seem to indicate that the valence electrons of the magnesium atom are completely ionized and that the small amount of charge accumulated between the magnesium sites comes from the boron atoms. Therefore, the magnesium atoms operate as a structural block separating the boron planes. But they do not make a noticeable contribution to the electronic properties of the material, in particular to the electrical conductivity, since there is no bonding between the magnesium atoms. These results are also corroborated by the analysis of the contributions to the DOS, where the magnesium atoms present a very small contribution, see Table 1; similar results were found by Kortus et al. [22].

From Fig. 3 one gets an impression of the behavior of the charge density along the line joining the magnesium and boron atoms. The character of the bond between these two atoms can now be inferred: it is highly ionic, with most of the charge shifted towards the boron atom, but with a small covalent component. This can be more clearly seen in Fig. 4c.

The B–B inter-planar distance is twice that of the nearest neighbor atoms lying in the plane. Therefore, most of the conductivity should be in the boron planes (a- and b-directions) and only a small contribution should occur between the planes (c-direction). The c-direction conductivity is expected to be mainly due to

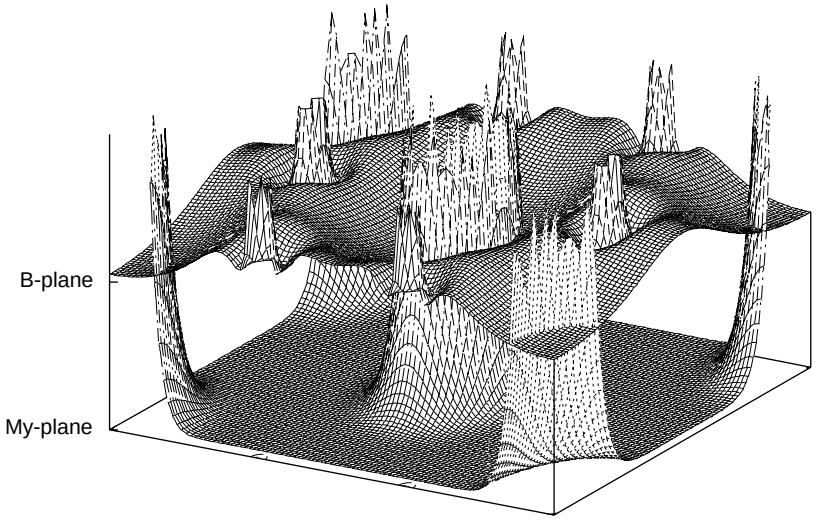

Fig. 1. Charge density plot for two planes of MgB_2, the lower plot corresponds to the magnesium plane, where the atoms are in a triangular arrangement. The upper plot (shifted upwards by 2 units for visibility reasons) corresponds to the boron plane, with the boron atoms forming a honeycomb array.

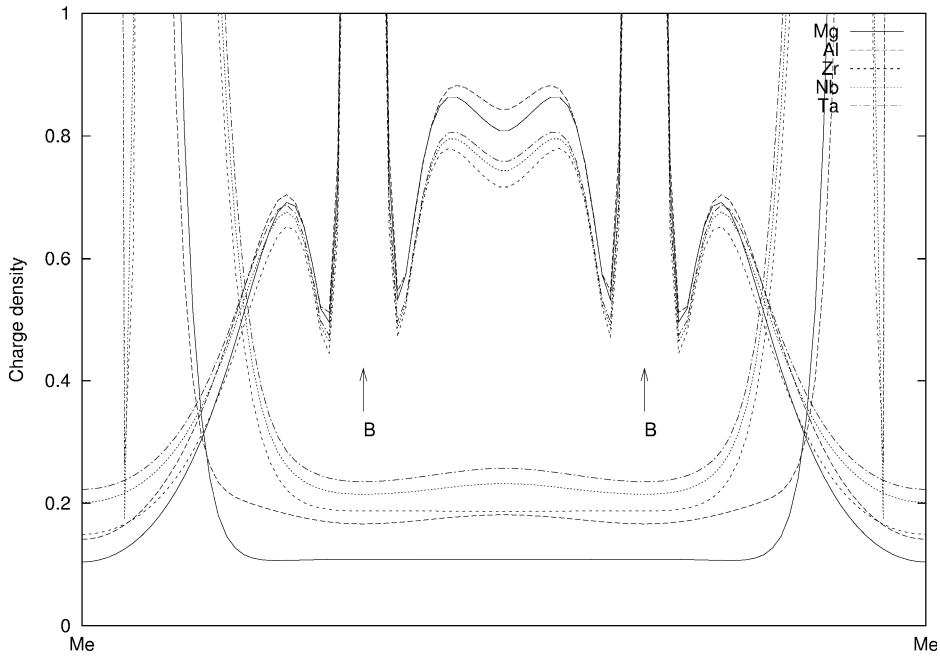

Fig. 2. Charge density profiles along two different crystal paths of MeB_2. The set defining a flat region corresponds to the line joining the $Me-Me$ second nearest neighbor atoms (Me = Mg, Al, Zr, Nb, and Ta). The other set is the one corresponding to a line in the boron plane, exactly above the first one. This second line crosses two nearest neighbor boron atoms. The plots for Me = Mg correspond to the forefront profile as seen from the left of Fig. 1, but the boron plot is not shifted upwards. Note that for the boron plane the extremes of the plot correspond to the center of the boron hexagons, where the density values are very close to the values at the Me plane.

Table 1
DOS values at E_F for the different MeB_2 compounds. The contributions of the Me and B atoms and of the interstitial region are indicated in percent. The Me/B DOS ratio is also shown

DOS	Mg	Al	Zr	Nb	Ta
Total	0.717	0.371	0.301	1.024	0.935
Me (%)	3.4	15.0	26.5	37.5	48.3
B (%)	44.5	23.6	16.4	16.9	19.7
Interst (%)	52.2	61.4	57.1	45.7	32.0
Me/B	0.075	0.64	1.62	2.22	2.46

the magnesium contribution. As discussed above, the Mg–B bond has a small covalent character which contributes little to the c-direction conductivity. Only an explicit calculation can quantify the different contributions, as will be discussed below.

4.1.2. MeB_2 (Me=Al, Zr, Nb and Ta)

Fig. 2 shows a clear B–B covalent bond formation, which is of similar magnitude for all the studied compounds. On the other hand, in the Me plane the charge density is not as flat as for the Mg compound, indicating that these metal atoms do not have the charge so tightly bound, and are therefore less ionized. The charge density values increase along the Mg, Al, Zr, Nb, and Ta sequence, with the curvature of the plots, except for ZrB_2, showing the same trend.

The flat charge density plot of ZrB_2, displayed in Fig. 4a is similar to MgB_2 and would suggest a similar behavior which seems to agree with the finding that ZrB_2 is a superconductor at 5.5 K [3]. However, this flat charge density behavior does no longer appear along the nearest neighbour line, as shown in Fig. 4b. Therefore, the calculated charge density would not predict a superconducting behavior for ZrB_2, the flat feature in Fig. 4a is only an accidental characteristic.

The charge density profiles reported in Fig. 4c clearly show how the $Me-B$ covalent bond character increases in the Mg, Al, Zr, Nb, and Ta sequence, suggesting that the σ_a/σ_c ratio should decrease in the same sequence. This will be discussed below.

5. Density of states

For the studied MeB_2 compounds, an analysis of the contributions to the DOS at E_F is shown in Table 1. It is clear that MgB_2 is quite different from the other compounds; since the relative contribution of the magnesium atoms is significantly smaller than that of the Me atoms in the other compounds. Even more, the boron contribution is much higher in MgB_2. This analysis reinforces our previous finding that the magnesium acts only as a dividing block between the boron planes, while in the other MeB_2 compounds the Me atoms contribute to the electrical conductivity.

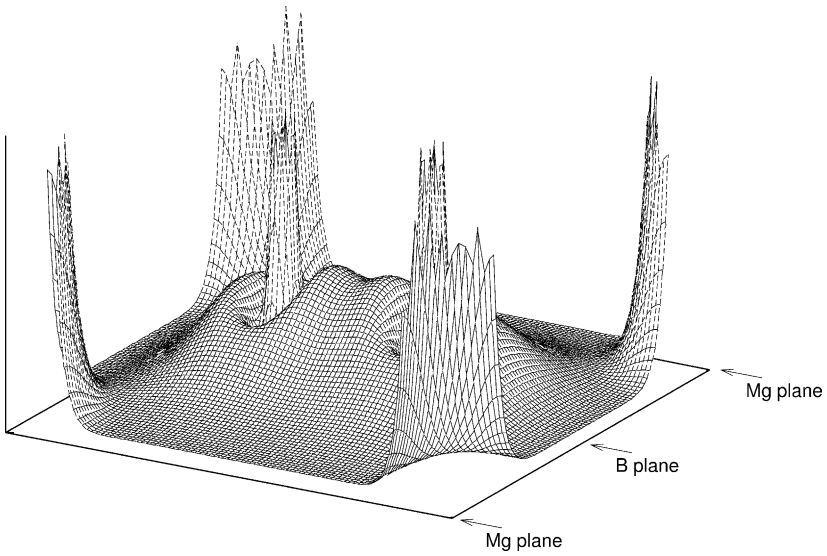

Fig. 3. Charge density on a vertical plane of MgB_2 defined by the two magnesium atoms of Fig. 2 and the corresponding ones in the next magnesium plane. This plane includes two boron atoms (at the center of the figure). In this figure the charge profiles of Fig. 2 can again be seen.

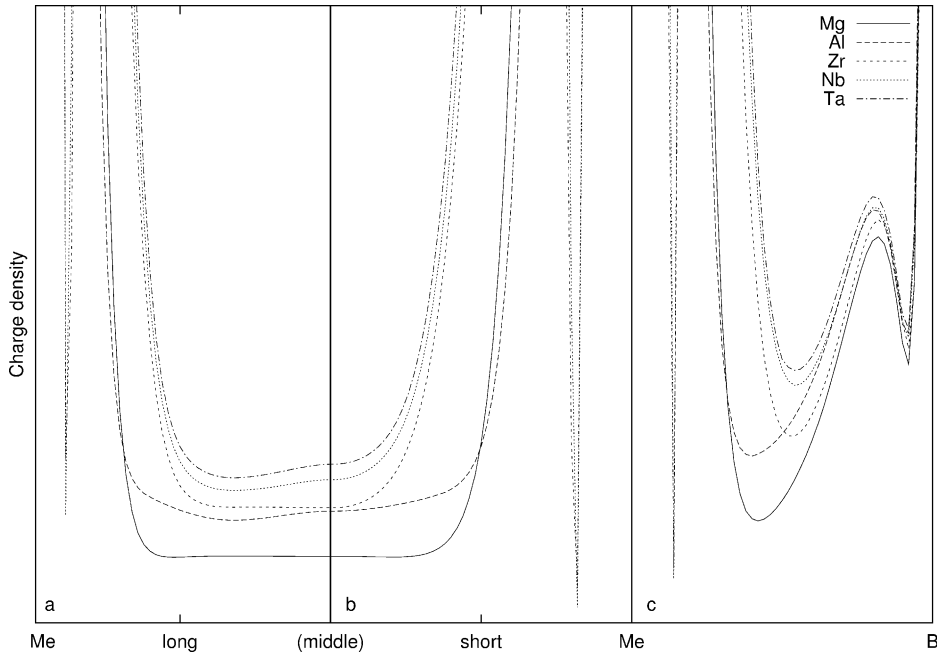

Fig. 4. Charge density along lines joining different atoms: (a) ρ along the line joining $Me-Me$ second nearest neighbors (due to symmetry only half is shown), (b) ρ along the line joining the $Me-Me$ first nearest neighbors (it corresponds to the view from the right of Fig. 1), and (c) ρ along the line joining $Me-B$.

These results seem to indicate a 2D electrical conductivity for the MgB_2 system and a bulk conductivity for the rest. Consistently, the Me/B ratio abruptly jumps by about a factor of 8.5 from MgB_2 to AlB_2; then, it continues with a more moderate increase in going towards the heavier *Me*. In this sequence the *Me* contribution increases continuously, while the boron contribution decreases at first but it levels out at the end. As mentioned above, E_F in MgB_2 is below a semi-gap (a low-density region), suggesting a hole character for the conductivity, while for the other compounds it is located above, suggesting an electron character. The semi-gap is narrower and deeper in the last three compounds.

The results discussed above reveal a trend in the Mg, Al, Zr, Ta and Nb sequence; the interstitial charge in the *Me* plane increases (Figs. 2 and 4); the curvature of this charge plot also increases and *Me* DOS contributions (Table 1) follow the same trend. The magnesium compound stands out from the rest, having the

following characteristics: there is a large difference in the DOS values, the interstitial charge in the Mg plane is flat, and it has the lowest value.

6. Band structure and electrical conductivity

The electrical conductivity can be calculated, in the relaxation time approximation, from band structure results, using the following expressions [23,24]:

$$\sigma_{\alpha\beta} = e^2 \int \frac{\mathrm{d}k}{4\pi^3}\tau(\varepsilon(k))v_\alpha(k)v_\beta(k)\left(-\frac{\partial f}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon(k)},$$

$$v_\alpha(k) = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k_\alpha}.$$

The anisotropy in these expressions comes entirely from the anisotropy of the Fermi surface anisotropy. At higher level of approximation, additional anisotropy enters from the anisotropy of the scattering, but from the cases studied by Allen and co-workers [25–27] this turns out to be a surprisingly small effect (a few percent), at least for electron–phonon scattering at $T \geqslant \theta_D$.

For a metal $-\partial f/\partial\varepsilon$ can be approximated by a delta function at E_F and $\tau(\varepsilon(k)) = \tau(\varepsilon_F, T)$ is now independent of $\mathbf{k}$ and can be taken out of the integral:

$$\sigma_{\alpha\beta} = \frac{e^2\tau(\varepsilon_F, T)}{4\pi^3}\int \mathrm{d}k v_\alpha(k)v_\beta(k)\delta(\varepsilon_F - \varepsilon(k)).$$

With $\mathrm{d}\mathbf{k} = \mathrm{d}S_\alpha \mathrm{d}k_\alpha$ (where $\mathrm{d}S_\alpha \perp \mathrm{d}k_\alpha$) this expression can be integrated in the $\mathrm{d}k_\alpha$ direction, and from the properties of the delta function reduces to

$$\sigma_{\alpha\beta} = \frac{e^2\tau}{4\pi^3\hbar}\int \mathrm{d}S_\alpha \sum_i \left|v_\beta^i(k_F)\right|,$$

where the summation over i is for all the bands at the Fermi energy.

With this expression the conductivity can be calculated, except for τ, from the band structure. τ contains all the temperature dependence, and what will be reported in this work is the relative conductivity, $\sigma_\alpha^r = 4\pi^3\hbar\sigma_{\alpha\alpha}/e^2\tau$. This term is related to the plasma frequency (w_p) and to the Fermi velocity (v_F) : $\sigma_\alpha^r = \pi^2 w_p^2/e^2 = 4\pi^2 N(\varepsilon)v_F^2$, where $N(\varepsilon)$ (shown in Table 1) is the DOS [24,28,27]. The temperature dependence of the conductivity has been reported, for MgB_2, by Putti et al. [29].

6.1. MgB_2

As it can be seen in Fig. 5a all the bands along the $a-b$ plane have a large slope at E_F. The bands in the c-direction that pass through $\Gamma(\Gamma-A)$ are doubly degenerated and horizontal, they have mainly $B : p_x + p_y$ character. On the other hand, the $L-M$ bands, also in the c-direction, have a large slope, they have a $B : p_z$ contribution but also a small Mg component. This slope indicates that there is a significant orbital overlap at E_F in the c-direction and that this material is a conductor in this direction. Therefore, the conductivity expressions could also be used in this case.

From these results it can be seen that the conductivity is large in the $a-b$ plane and comes mainly from the boron honeycomb sublattice. In the c-direction, the $\Gamma-A$ bands are largely insulating, but the $L-M$ bands are not. From these considerations, it is clear that the conductivity in the c-direction is smaller than in the $a-b$ plane but not negligible. The small magnesium and $B : p_z$ contributions in the $L-M$ bands also suggest that there is a conductivity along the B–Mg bonds. The conductivity ratio, calculated from the above equation, is $\sigma_a^r/\sigma_c^r = 4.74$ (see Table 2). This value is large but the material is not an insulator in the c-direction as some high T_c superconductors [30,31]. Therefore, this material is a 3D conductor!

6.2. MeB_2 (Me=Al, Zr, Nb and Ta)

All compounds, including MgB_2, have the same crystal structure and the general features of the band structure should be the same, differing only in details.

The observed trend is that there is a continuous shift upwards in E_F going from Al to Ta since the metal atom contributes more electrons to the crystal. Nb and Ta have the same valency and have similar features. The magnesium and aluminum compounds have a very similar band structure, this is mainly because Mg and Al are both sp metals. However E_F for AlB_2 is ≈ 2 eV higher and crosses different bands; those at $\Gamma-A$ now have a large slope, increasing σ_c and reducing the conductivity ratio, which is now $\sigma_a/\sigma_c = 2.92$ (in contrast to 4.74 for MgB_2).

The rest of the compounds, those containing transition metal atoms (Zr, Nb and Ta), have a similar band structure among themselves, but different from that of Mg and Al. In particular, the bands near E_f in the c-direction, are no longer flat, see Fig. 5. Since Nb and Ta are isovalent E_F has almost the same relative energy in the band structure, but it is about 2 eV higher relative to the band structure of ZrB_2.

As mentioned, the band structures can be grouped in two sets [Mg, Al] and [Zr, Nb, Ta], containing metals with sp and sd valence electrons, respectively. This division can also be observed in the charge density profiles, displayed in Fig. 4. Indeed, the *Me-sp* densities follow a different pattern than the *Me-sd* ones.

As reported in Tables 1 and 2, the σ_a/σ_c ratio is inversely proportional to the relative *Me*-DOS value. This result suggests that the *Me* charge plays an important role in the electrical conductivity anisotropy.

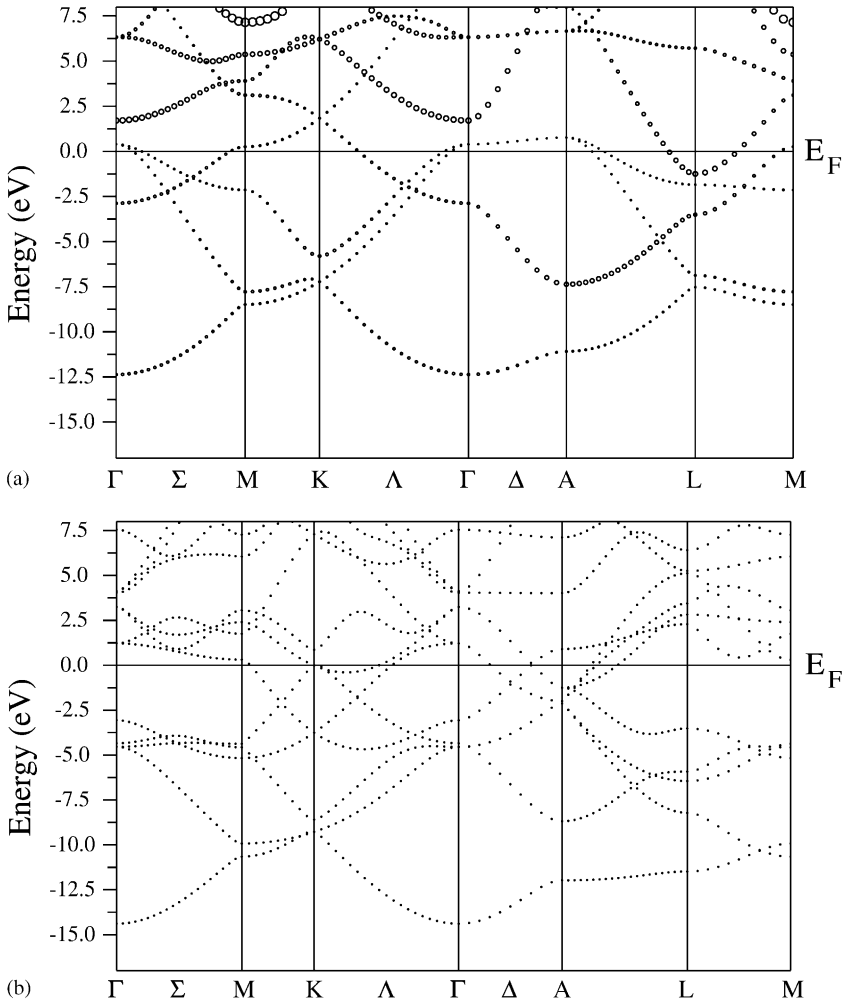

Fig. 5. Band structure of (a) MgB_2 (b) NbB_2. $\Gamma-M-K-\Gamma$ and $A-L$ correspond to the a–b plane and $\Gamma-A$ and $L-M$ are on the c-direction. In MgB_2 the size of the circles indicates the magnesium contribution. Notice that, in this graph, this contribution is always small; the corresponding graph for boron, not shown here, has substantially larger circles.

Table 2
Relative conductivity values $\sigma_\alpha^r(=4\pi^3\hbar\sigma_{\alpha\alpha}/e^2\tau)$ for the different MeB_2 compounds. The relaxation time τ was taken the same for the different compounds since the conductivity is mainly due to the boron sublattice

Conduct.	Mg	Al	Zr	Nb	Ta
σ_a^r	0.326	0.454	0.088	0.251	0.292
σ_c^r	0.069	0.155	0.034	0.106	0.127
σ_a^r/σ_c^r	4.74	2.92	2.61	2.37	2.29

7. Conclusions

In MgB_2, the magnesium atoms, as expected, have the outer s electrons almost completely ionized and form an almost ionic bond with boron, with a very small covalent contribution. In the magnesium plane there is no Mg–Mg bond. In contrast, in the boron planes the B–B bonding is quite strong and covalent.

When magnesium is replaced by Al, Zr, Ta or Nb, the character of the boron–boron bond shows little variation, while the $Me-B$ bond increases its covalent character, but still remains highly ionic. On the other hand, the $Me-Me$ bond (in the Me planes) begins to show an increase of charge in the $Me-Me$ internuclear region, indicating the appearance of a small covalency.

The band structures of this set of metal borides have essentially the same features. The main differences result from a shift of the Fermi level and the increase of the valence electrons. This has noticeable effects on the dimensionality of the conductivity and on the participation of Me in this process.

There is a qualitative difference between MgB_2 and the other compounds. In the non-magnesium compounds the Me atoms keep significantly more charge outside their core and those electrons participate in the conductivity in the a–b directions. The charge density in the Me plane is flat for MgB_2. This feature is lost in the

other compounds, with an increasing curvature in the charge density along the Al, Zr, Nb and Ta sequence.

MgB_2 exhibits a strong 2D character in the charge density, but it is still a 3D electrical conductor, as indicated by the conductivity ratio. The 3D character of the conductivity in MgB_2 could be indicative of a low flux pinning effect.

It was expected that a 2D electrical conductivity in MgB_2 could contribute to the superconducting electron–electron coupling, but the low conductivity anisotropy rules out this possibility.

The difficulty of the *c*-direction electrical conductivity measurements makes the theoretical calculations of the conductivity almost the only possibility for the prediction of this property.

The almost completely ionic character of the Mg–B bond, with an internuclear separation of 2.505 Å, as compared to the short and covalent B-B bond (1.781 Å), makes the in-plane boron phonons strong and independent from the magnesium planes. Note that, aside from the big Mg–B separation, a covalent bond is more rigid and directional. This effect would be smaller in the other $Me-B_2$ compounds due to the larger covalent character of the $Me-B$ bond, therefore superconductivity in these latter compounds, as reported for ZrB_2, would be of a different nature. On the other hand, this effect should be more pronounced in LiBC, since the Li–B and Li–C bonds would be even more ionic (less covalent) than the Mg–B bond. If this compound can be made superconducting by hole doping [32], then, the above mechanism would work even better.

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