Critical Temperature $T_c$ and Charging Energy $E_c$ between B-B layers of Superconducting diboride materials MgB$_2$ in 3D JJA model

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The diboride materials MB$_2$ (M= Mg, Be, Pb, etc.) are discussed on the basis of the 3D Josephson junction array (JJA) model due to Kawabata-Shenoy-Bishop, in terms of the B-B layers in the diborides analogous to the Cu-O ones in the cuprates. We propose a possibility of superconducting materials with the MgB$_2$-type structure which exhibit higher critical temperature $T_c$ over 39K of MgB$_2$. We point out a role of interstitial atomic ions (e.g., Mg in MgB$_2$) as capacitors between the B-B layers, which reduce the charging coupling energy in JJA.

KEYWORDS: MgB$_2$, Josephson Junction Array model, Ionic electronic polarizability, Charging energy

Since Akimitsu and co-workers presented a remarkably high temperature (≈39K) superconducting magnesium diboride material MgB$_2$ in the beginning of 2001, much attention has been focused on studying the diboride material superconductivity. The material MgB$_2$ takes the layered structure of B-Mg-B stacking and has a coupling between 2-dimensional (2D) B-B layers. It is believed from several band calculations, that in the MgB$_2$-type crystal structure there exist a strong covalent B-B bonding and an ionic B-Mg bonding. The strong covalent B-B bonding and the presence of the ionic Mg atoms lead to hole-like cylindrical Fermi surfaces in MgB$_2$ and the holes are conducted in each 2D B-B layer. It is observed that the 2D B-B layers, like the Cu-O layers in high-$T_c$ cuprates, play an important role in the electrical transport properties. MgB$_2$ can then be a beautiful realization of the essential physics of superconductivity in cuprates, without the complications of Cu $d_{x^2−y^2}$ orbitals.

In this short note, in terms of a theoretical model of the B-B layers analogous to the Cu-O layers, we propose a possibility of superconducting materials of the MgB$_2$-type structure with higher critical temperature $T_c$ over 39K. We point out an important role of interstitial atomic ions (e.g., Mg in MgB$_2$) as capacitors between the layers.

We model the diboride MB$_2$ materials (M= Mg, Be, etc.) as quantum-capacitive Josephson junction arrays (JJA) with weakly coupled superconducting grains on a 3D lattice and angstrom-scale parameters, following Kawabata-Shenoy-Bishop (hereafter, we call KSB) theory. Originally proposed to the high-$T_c$ cuprates with 2D Cu-O layers and a coupling between the Cu-O layers. It means that the Josephson junction coupling energy $E_j$ via the Cooper pair tunneling within and between the B-B layers enhances the critical temperature $T_c$ for layered B-B superconductors, while the charging coupling energy $E_c$ between the B-B layers depresses $T_c$. The origin of $E_c$ is that, when the Cooper pairs tunnel between the layers, local inter-layer charge imbalance is induced between the superconducting grains in JJA. Here, the interstitial ionic atoms, M, located between the B-B layers play a role of capacitors, reducing the charging coupling energy $E_c$ by the electric polarization of the ionic atom.

Referring to Kittel’s textbook and Shockley’s table, for the ionic radii $d$ and electronic polarizability $\varepsilon$ of the ionic atoms M, we have obtained the charging coupling energy $E_c ∼ d/\varepsilon$ between the B-B layers in Table 1 following the KSB theory. By hypothesizing same Josephson junction coupling energy $E_j$ within the B-B layers for any diboride materials, we estimate critical temperatures $T_c (= f(E_c))$ considering the competition between the Josephson junction coupling energy $E_j$ and the charging coupling energy $E_c$ for the diboride compounds MB$_2$. We here discuss, by way of illustration, the ion compounds M$^{2+}$(B$^{-}$)$_2$ expected to have nearly the same electronic structure as MgB$_2$ (Mg$^{2+}$(B$^{-}$)$_2$), and then to have almost the same $E_j$ (i.e., a “bare” $T_c$) without any influence of the M-atom-dependent charging coupling energy $E_c$.

In Fig. for the $E_c$ vs. $T_c$ plot, we show two points, an experimentally known data, for BeB$_2$ ($T_c ≃ 0K (< 5K)$), $E_c = 43.75$) and MgB$_2$ ($T_c = 39K, E_c = 6.91$), where $E_c (∼ d/\varepsilon)$ are of Table 1 and in arbitrary units. These two are, at present, the only reported materials with the MgB$_2$-type structure on which $T_c$ are measured experimentally. While only two points have been determined so, we draw a straight line (solid line) as is shown in Fig. 1 assuming simple linear relation, $T_c = f(E_c) ∼ E_j − E_c$. We see that, when this solid line crosses the $T_c$-horizontal axis, such a $T_c$-cross-point seems to be larger than 39K. For various diboride compounds with different $E_c$ in Table 1, data points align on the line in Fig. 1, and then $T_c$ can be estimated for each compound. From this graph, for compounds which have smaller $E_c$ than MgB$_2$, $T_c$ higher than 39K of MgB$_2$ are obtained. That is, since $E_c$ of the ionic atoms in Table 1 except for Be$^{2+}$, are smaller than that of Mg$^{2+}$, higher $T_c$ is estimated for various MB$_2$ compounds owing to the relation $E_c = f^{-1}(T_c)$ as shown by the line in Fig. 1. Especially for the compound containing the Pb atom, high $T_c$ is expected because of large polarizability $\varepsilon$ (thus, small $E_c$) of the ionic Pb in Table 1.
We represent, in what follows, two kinds of possibility that \( T_c \) may become higher than those estimated from the solid line drawn in Fig. 1. One possibility is that, if \( E_j - E_c < 0 \) for BeB\(_2\), which means it never exhibits superconductivity, i.e., \( T_c = 0 \), then we infer that the \( E_c \) vs. \( T_c \) plot becomes a line with a smaller slope as shown by the dashed line in Fig. 1 because a (virtual) \( T_c \sim E_j - E_c \) for BeB\(_2\) is negative on the graph of Fig. 1 in this case. The other is that, while we have assumed the function \( f(E_c) \) or \( f^{-1}(E_c) \) as a linear line, it can be a curve with positive curvature in general. A curve, \( E_c = f^{-1}(T_c) \), with positive curvature which goes through both the points for MgB\(_2\) and BeB\(_2\) in Fig. 1, could give rise to rather higher \( T_c \) in the region of small \( E_c \). We then expect that the critical temperatures \( T_c \) could be possible to reach up to the region over 77K, the evaporation temperature of liquid nitrogen.

In conclusion, we indicate that, if MgB\(_2\)-type compounds are synthesized by using ionic atoms with larger polarizability or smaller diameter instead of the Mg atoms, the critical temperatures \( T_c \) would become higher. We hope that the present proposal is an encouragement to the synthesis of compounds and new high-\( T_c \) superconducting systems over 39K with the MgB\(_2\)-type structure will be discovered in the near future.

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### TABLE I. Ionic radii \( d \) (from ref. 15), ionic electronic polarizability \( \varepsilon \) (from ref. 16) and charging coupling energy \( E_c \sim d/\varepsilon \). The data of \( \varepsilon \) in brackets are of ref. 17 originally and the value of \( d \) for Cu\(^{2+}\) is of ref. 18.

| Ion     | Ionic atom radii \( d \) [10\(^{-8}\)cm] | Ionic electronic polarizability \( \varepsilon \) [10\(^{-24}\)cm\(^3\)] | Charging coupling energy \( d/\varepsilon \) \( E_c \) | Critical temperature \( T_c \) [K] |
|---------|---------------------------------|---------------------------------|---------------------------------|-----------------|
| Be\(^{2+}\) | 0.35 (0.008) | | (43.75) | 39 |
| Mg\(^{2+}\) | 0.65 (0.094) | | (6.91) | 39 |
| Ca\(^{2+}\) | 0.99 (0.47) | | (2.11) | 39 |
| Sr\(^{2+}\) | 1.13 (0.86) | | (1.31) | 39 |
| Ba\(^{2+}\) | 1.35 (1.55) | | (0.87) | 39 |
| Zn\(^{2+}\) | 0.74 (0.8) | | 0.93 | 39 |
| Cd\(^{2+}\) | 0.97 (1.8) | | 0.54 | 39 |
| Cu\(^{2+}\) | 0.72 (0.2) | | 3.60 | 39 |
| Pb\(^{2+}\) | 0.84 (4.9) | | 0.17 | 39 |

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