Crystal Chemical Estimation of possible exceeding of $T_c \leq 77$ K in Diborides

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Abstract

We establish the empirical correlation between $T_c$ of diborides (AB₂) and crystal chemical parameters of simpler structural fragment – sandwich A₂(B₂) where the superconductivity is appeared, like found in high-$T_c$ cuprate superconductors. Our results suggest that in the absence of vacancies in B₂ plane $T_c$ of diborides can be higher 77 K, the evaporation temperature of liquid nitrogen. We discuss critical crystal chemistry parameters controlling $T_c$ and ways to achieve higher transition temperatures in diborides based on this correlation.

Key words: diboride; MgB₂; superconducting transition temperature; crystal chemical correlation.

1. INTRODUCTION

Attempts to exceed the temperature of transition to superconductivity ($T_c$) 39 K [1] in the AB₂ diborides row with the AlB₂ structure have until no success. However, the presence of some common crystal chemical characteristics in diborides and high-temperature superconductor cuprate (HTSC) cuprates allows to expect that possibility of raising $T_c$ in these compounds still exist. Intensive study of MgB₂ had shown that as in HTSC cuprates the layered nature of MgB₂ is caused anisotropic superconducting properties [2, 3]. It was shown that $T_c$ of MgB₂ either as in HTSC cuprates depends on the concentration of charge carriers [4, 5] and structural parameters [6, 7]. The similar ways of variation in concentration of charge carriers and structural parameters by isovalent and non-isovalent doping [7, 8-15] and by pressure [5, 16-23] also were considered. It was
established that in diborides the B₂ planes contain such carriers of charge as holes (p) and play the same role as the CuO₂ in high-$T_c$ cuprates [4, 24, 25]. In AB₂ these planes there are between the planes of positive charged “ions” A, as the CuO₂ planes in perovskite layer $A_{n+1}(CuO_2)_n$. Note, that in the last this is reached for account of displacement or full removing the apical oxygen atoms from plane of A cations on consequence of Jan-Teller effect.

In [26] we have shown that the simplest structural fragment in HTSC cuprates is not one CuO₂ plane but $A_2(CuO_2)$ sandwich, in which the CuO₂ plane with charge carriers is situated between the planes of A-cations, and have installed the correlation of $T_c$ with critical crystal chemical parameters of this sandwich general for all phases of HTSC cuprates. It is possible to expect that in diborides AB₂ of such structural fragment is the $A_2(B_2)$ sandwich, where the network of B atoms with charge carriers is situated between the planes of A “cations”.

In this work we consider a dependence of $T_c$ from crystal chemical parameters of $A_2(B_2)$ sandwich in diborides like found in HTSC cuprates and discuss the possibilities and ways to rise $T_c$ in this class of compounds.

2. METHOD

In high–$T_c$ cuprates $T_c$ dependence on crystal chemical parameters of the $A_2(CuO_2)$ fragment is more full expressed by combination of such values as distances $d(Cu-Cu)$ in CuO₂ plane and ones $d(CuO_2-A)$ from CuO₂ plane to adjacent plane of A cations, which have an original sense and give also an information about the hole concentration, and on the size and charge of A-cations and doping atoms too. In [26] we established the empirical dependence of $T_c$ from the ratio ($J$) of distances between Cu atoms along diagonal direction of CuO₂-plane to sum “effective” distances $(D_1+D_2)$ from CuO₂ plane to of two adjacent planes of A cations in $A_{n+1}(CuO_2)_n$ layer, taking into account the charge and the size of A-cations and doping atoms ($J = d(Cu-Cu)/(D_1+D_2)$).

For plotting the dependence of $T_c(J)$ in AB₂ where

$$J = d(B-B)/(D_1 + D_2)$$  \hspace{1cm} (1)$$

we have chosen critical parameters of $A_2(B_2)$ fragment, like found in high–$T_c$ cuprates, such as:

1. The $d(B-B)$ distances between B atoms situated at the ends of diagonal of hexagons in B₂ plane ($d(B-B) = 2a/\sqrt{3}$), i.e., at the maximal possible distance from one another. It is supposed, that the diagonal pairing and oscillation of holes on B atoms are energetically more favourable than other configurations [27];
2. “Effective” distances \( D_1 \) and \( D_2 \) from \( B_2 \) plane to surface of two adjacent planes of \( A \) “cations”:

\[
D = 5\left[ d(B_2 - A) - R_A(Z_A/2) \right]
\]

where \( d(B_2 - A) \) is the distance from \( B_2 \) plane to plane of \( A \) “cations”; \( R_A \) is radius of \( A \) “cation”, which content is maximum; \( Z_A/2 \) – undimensional coefficient to take into account of the electric field of the \( A \) “cation” charge (it is the ratio of charge \( A \) “cation” to charge of Mg cation), \( S \) is deviation coefficient of parameters of doping cations from parameters of \( A \)-cation that forms the plane:

\[
S \geq 1, \ S = \frac{R(Z/2)}{R_A(Z_A/2)} \quad \text{or} \quad S = \frac{R_A(Z_A/2)}{R(Z/2)}
\]

Here \( \overline{R(Z/2)} \) is generalized value, characterized the plane of \( A \)-cations:

\[
\overline{R(Z/2)} = m_1 R_{Z_1}(Z_{Z_1}/2) + ... m_n R_{Z_n}(Z_{Z_n}/2)
\]

where \( m_n \) is content of \( A_n \) “cation” in plane, \( R_{Z_n} \) is radius, \( Z_{Z_n}/2 \) – undimensional coefficient to take into account of the electric field of the \( A_n \) “cation” charge.

On value \( J \) an enormous influence renders a size and a charge (valence states) of \( A \) “cations”. To value these parameters in intermetal compounds is not easy. By interpretation the result on diborides practically in all works the Pauling “crystal” ion radii are used [28]. However, this system reflects inadequately the changing of a lattice parameter \( c \) by changing a radius of \( A \) “cations”. So, lattice parameter \( c \) of \( AlB_2 \) (3.26 Å) is noticeable less than \( c \) parameter of \( MgB_2 \) (3.52 Å) [29]. Pauling radii \( (RP) \) Al (0.75 Å), opposite, exceeds a radius of Mg (0.65 Å). Proceeding from approximately linear correlations between \( c \) parameters of diborides and \( A \) radius the Shannon crystal radius \( (RSh) \) is more suitable. In Fig. 1, lattice parameters \( c \) are plotted as a function of Shannon (a) and Pauling (b) radii of \( A \) “cations”. However, \( J \) was calculated by using both Pauling and Shannon radii systems with standard coordination 6 and valent state equal group number in Periodic system, excluding Mn, Cr, Ru and Os. The valent state of Mn and Cr was accepted as 4+ and 3+, accordingly, but Ru and Os as 6+. Moreover, Ru radius was accepted such as for Os, as there is no data about Ru radius.

Besides, for the plotting of \( T_c(J) \) it is necessary to know \( T_c \) of sample and its full structural data (atomic coordinates and occupancy positions) obtained by X-ray and neutron diffraction. It is not sufficiently the only data about unit cell parameters, as the vacancies in \( A \) plane can change a \( J \) value and, accordingly, \( T_c \) but the vacancies in \( B_2 \) plane, as in \( CuO_2 \) plane of HTSC cuprates, reduce \( T_c \) or suppress completely a superconductivity. Besides, the impurities in \( A \)-planes can be distributed
irregularly along the c axis, as that was shown in [13] for Mg\(_{1-x}\)Al\(_x\)B\(_2\) by high-resolution transmission-electron microscopy investigation. This will certainly result in a change and inequality of “effective” distances \(D_1\) and \(D_2\), accordingly, and to change \(J\) and superconducting characteristics. There isn’t now such data on doping borides.

Realistically it is installed only the following:

1. Crystal structure of diborides, lattice parameters and \(T_c\) of polycrystalline and thin films of many MgB\(_2\) samples [1, 5, 7, 31-35], and the structural data obtained by X-ray diffraction analysis on single crystal of only one MgB\(_2\) sample [36], as well as the lattice parameters and the absence of superconductivity in AlB\(_2\)[10, 12, 13];

2. Reducing of MgB\(_2\) \(T_c\) with the growing of pressure (P). Moreover the spread of \(dT_c/dP\) reported by different groups [5, 16-23] is high and is explained in [21] by various in the sample stoichiometry.

3. The substitution of Al for Mg in MgB\(_2\) decreases the \(T_c\) and leads to the loss of superconductivity in Mg\(_{1-x}\)Al\(_x\)B\(_2\) with the growing \(x\) [7, 10-13].

It has been also found the superconducting transition at \(T_c=9.5\) K for TaB\(_2\) [37, 38] and no superconducting for TiB\(_2\), HfB\(_2\), ZrB\(_2\), VB\(_2\) and NbB\(_2\). Although this result contradicts the data reported in [39], by which ZrB\(_2\) is superconducting with \(T_c=5.5\) K, and TaB\(_2\) and NbB\(_2\) are not. Further to this we have the experimental and theoretical data on superconductivity and structural properties of Mg\(_{1-x}\)A\(_x\)B\(_2\) (A = Al, Zn, Ca and Na [7-13, 40] and only structural parameters of the other members of the AB\(_2\) family (A = Ru, Os, Cr, Mn, Mo, W, V, Nb, Ta, Ti, Zr, Hf, Sc, Y, Cu, Ag, Au, Lu, Pu and U) [29, 41-62] on superconducting properties of which not yet made final conclusions.

In this connection we have calculated two variants of \(T_c(J)\) correlation: with only real data for compounds MgB\(_2\) (single crystal) [36], AlB\(_2\) [29, 57] and disputable data on TaB\(_2\) [37] or ZrB\(_2\) [39]. The both systems of radii (\(R_{Sh}\) and \(R_P\)) were used by this calculation. As a result we have got two correlations for the variant-I (\(T_c^{Ta, R_{Sh}}(J_{R_{Sh}})\) and \(T_c^{Ta, R_P}(J_{R_P})\) (Fig. 2 a)) and two correlations for variant-II (\(T_c^{Zr, R_{Sh}}(J_{R_{Sh}})\) and \(T_c^{Zr, R_P}(J_{R_P})\) (Fig. 2 b)). The equations of second degree polynomial give the best approximation of the correlations:

\[
T_c^{Ta, R_{Sh}} = -6.05213 J_{R_{Sh}}^2 + 169.383 J_{R_{Sh}} + 95.324, \text{ there midpoint } J_0 = -1.30395, T_{c, \text{max}} = 107; \quad (5)
\]

\[
T_c^{Ta, R_P} = -9.93835 J_{R_P}^2 - 68.1881 J_{R_P} + 173.101, \text{ there midpoint } J_0 = -3.38595, T_{c, \text{max}} = 290; \quad (6)
\]

\[
T_c^{Zr, R_{Sh}} = 1.21806 J_{R_{Sh}}^2 - 51.7357 J_{R_{Sh}} + 135.714, \text{ there midpoint } J_0 = 20.8830, T_{c, \text{min}} = -413; \quad (7)
\]
\[ T_c^{Zr,RP} = 11.0727 J_R^{2} - 143.304 J_R + 239.537, \text{ there midpoint } J_0 = 6.3148 \text{ } T_c, \text{min} = 224; \]  

(8)

Then, for the estimation of validity of these two correlation variants \( J_{RSh} \) and \( J_{RP} \) by formula (1) and corresponding them \( T_c \) on equations (5-8) for 100 considered diborides were calculated. It was found that parabolic dependencies \( T_c^{Ta,RSh}(J_{RSh}) \) and \( T_c^{Ta,RP}(J_{RP}) \) of Eq. 5 and 6 obtained on the data for MgB\textsubscript{2}, AlB\textsubscript{2} and TaB\textsubscript{2} estimate adequately a trend of changing \( T_c \) of MgB\textsubscript{2} with the growing of pressure, and Mg\(_{1-x}\)Al\(_x\)B\textsubscript{2} with \( x \) increase, and confirm also an absence of superconductivity in ZrB\textsubscript{2} [37] (Table I). However, a velocity of linear falling \( T_c \) \((dT_c/dP \text{ and } dT_c/dx) \) calculated on these correlations is more below than experimental [7, 10-13]. Moreover, according the data, obtained by these correlations, a very small changing of lattice parameters can result in the lost of superconductivity in TaB\textsubscript{2}. So, TaB\textsubscript{2} (Table I, sample N 28) in which the authors [39] did not find a superconductivity, by calculations on correlation \( T_c^{Ta,RP}(J_{RP}) \) of Eq. 6 also is not a superconductor, but on correlation \( T_c^{Ta,RSh}(J_{RSh}) \) of Eq. (5) it must be superconductor with \( T_c = 7.4 \)K. Here and further the number of compound in Table I is parenthetically shown. The calculation of \( T_c \) for TaB\textsubscript{2} (N 29 [29, 44] and N30 [54]) with increasing parameter \( c \) points to the absence of superconductivity by both correlations.

Correlations \( T_c^{Zr,RSh}(J_{RSh}) \) and \( T_c^{Zr,RP}(J_{RP}) \) of Eqs. (7) and (8) built with of using of data on ZrB\textsubscript{2} [39], probably, have no physical sense, as fare as it is impossible to explain a sudden disappearance and appearance of superconductivity. Besides, \( T_c \) calculated on the base of these correlations disagree to experimental data this work [39], as far as indicates not on the absence but opposite on the presence of superconductivity with unrealistic high \( T_c \) for diborides Nb, Ta and W, V, Hf, Pu, U also.

Thereby, a estimation has shown that the correlations of \( T_c^{Ta,RSh}(J_{RSh}) \) and \( T_c^{Ta,RP}(J_{RP}) \) are the most reliable. However, its can show only a trend \( T_c \) change with changing of crystal chemical parameters of diborides, as for its building there was too little experimental data. The \( T_c \) calculated on these correlations are referred to the diborides of stoichiometric composition, since there was no data for the account of non-stoichiometry of compounds by \( J \) calculation, while the last studies [16, 63, 64] point to Mg-deficiency and defects even in MgB\textsubscript{2}. As a result, calculated \( T_c^{Ta,RSh} \) of MgB\textsubscript{2} are little below than \( T_c \) found experimentally \((T_c^{exp})\). However, deficit of Mg (0.8, 0.9 and 1\%) in samples, N54, 59 and 53 (Table), accordingly, raises \( T_c^{Ta,RSh} \) \((38.1 – 38.3 \)K) calculated on the Eq. (5) to the experimental values \((38.8 – 39 \)K).
3. RESULTS AND DISCUSSION

Maximal $T_c$ values for diborides, calculated on correlation of $T_c^{Ta.RSh} (J_{RSh})$ and $T_c^{Ta.RP} (J_{RP})$ (Eqs. (5) and (6)) are 107 K at optimal value $J = J_0$ (by $J_0 = -1.304$) and 290 K (by $J_0 = -3.386$), accordingly. Increasing $T_c$ of diborides $AB_2$ by nearing $J$ to $J_0$ (Fig. 2 a) on the left occurs by shortening the distances $d(B-B)$ in $B_2$ plane and “effective” interplanar distances $D_1$ and $D_2$. (As on the given interval $D_1$ and $D_2$ have negative values the modules $D_1$ and $D_2$ must increase). This is possible from shortening the lattice parameters $a$ and $c$, reducing a size of A atom and increasing its charge. Moreover, the most effect is reached when a charge of atom is increasing. So, WB$_2$ (N5) has the most high $T_c$ (99.7 K and 290 K according to correlations $T_c^{Ta.RSh} (J_{RSh})$ and $T_c^{Ta.RP} (J_{RP})$) amongst considered diborides with $J < J_0$.

Besides, to rise $T_c$ of diborides with $J < J_0$ is possible by increasing $S$ coefficient to the account of introduction of vacancies in A layer or partial substitution A on the ions of smaller size or insignificantly differing from the size, but having smaller charge. For instance, $T_c$ of WB$_2$ and MoB$_2$ raise is possible by doping of W and Mo planes with the ions Ru$^{4+}$, Os$^{4+}$, V$^{5+}$, Ti$^{4+}$ (N18), Nb$^{5+}$ (N17) or Al$^{3+}$, but for TaB$_2$ by doping of Ta plane with Al$^{3+}$ (N34), Ti$^{4+}$ (N33) or V$^{5+}$ (N31) ions. For arising a superconductivity in NbB$_2$ it is necessary to introduce Nb-vacancies or substitute part of Nb$^{5+}$ on Al$^{3+}$ (N41), Ti$^{4+}$ or V$^{5+}$ (N42). The $T_c$ of diborides with $J < J_0$ must increase under the action of pressure, unlike MgB$_2$, where $J > J_0$.

However, superconductors with $J < J_0$, having high $T_c$, are hitherto not discovered. As it is mentioned above, TaB$_2$ is a superconductor at $T_c = 9.5$ K [35]. Cooper at al. [65] reported also, that in “boron-rich” NbB$_2$ compounds a superconductivity appears at $T_c = 3.87$ K, and in Zr$_{0.13}$Mo$_{0.87}$B$_2$ at $T_c = 11$ K. To our regret, the work [65] is inaccessible for us, but if expect that by substituting Mo on 13% Zr the lattice parameters $a$ and $c$ enlarged to 3.08 Å and 3.32 Å, accordingly, and there are no vacancies in B$_2$ plane, $T_c$ of Zr$_{0.13}$Mo$_{0.87}$B$_2$, calculated on Eq. (6) and Eq. (5) are 11 K and 86 K, accordingly.

Probably, a boron deficit in plane B$_2$ is a reason of absence of superconductivity in the diborides with $J < J_0$. It is possible a compression of a parameter caused by reducing a size of «cation» A can rezult in arising the vacancies in plane B$_2$. Consequently, a decrease $T_c$ of compound appears up to full suppress its superconductivity. On the contrary, substitution in
MoB$_2$ of part of Mo$^{6+}$ ions on large Zr$^{4+}$ ions with lower charge allows to obtain “boron-rich” diboride Zr$_{0.13}$Mo$_{0.87}$B$_2$ that is a superconducting properties. A problem appears to conserve a stoichiometry in B$_2$ plane in the diborides AB$_2$ with \( J < J_0 \) for the achievement of high \( T_c \). May be, this can be reached only by partial substituting A on more large “cations” with the lower charge. Such substitution reduces \( T_c \) that takes place in initial diborides but allows to obtain the superconductors with sufficiently high \( T_c \). Dopants saving stoichiometry on boron for AB$_2$ (A = W, Mo, Ru or Os) can be the following cations: Pb$^{2+}$, Mg$^{2+}$, Ag$^{2+}$, Sc$^{3+}$, Y$^{3+}$, Zr$^{4+}$, Sn$^{4+}$, Pb$^{4+}$, U$^{4+}$ and Th$^{4+}$.

In diborides with \( J > J_0 \), unlike diborides with \( J < J_0 \), \( T_c \) increase, when \( J \) nears to \( J_0 \) on the right, occurs not with reducing but with increasing “effective” interplanar distances \( D_1 \) and \( D_2 \). By this as well as in the diborides with \( J < J_0 \) the \( d(B-B) \) distances must decrease or its increase is more slow than \( D_1 \) and \( D_2 \) raising. This can be reached by increasing \( c \) lattice parameter with heightening the sizes of main or doping atoms of A plane and/or a \( S \) coefficient to the account of introducing the vacancies in A plane or partial substitution A on the ions of greater size or ones insignificantly differing from the size but with another charge. Experimentally proved [7, 10-13] that substituting Al on Mg in AlB$_2$ results in arising superconductivity and increase \( T_c \) to 39K in Al$_{1-x}$Mg$_x$B$_2$ with \( x \) growing. This substituting is accompanied with reducing \( J \) by in overtaking growing of interplanar distances \( D_1 \)and \( D_2 \) (N 80-88).

Usually inverse processes are considered, i.e. the suppress of superconductivity in MgB$_2$ by substituting Mg on Al or by pressing. Using the structural parameters from works [7, 17, 18, 40] we calculated the change of \( T_c \) of MgB$_2$ from pressure (N70-79) and Mg$_{1-x}$Al$_x$B$_2$ from \( x \) parameter (N 80-88). In both events \( J \) increasing, accompanied by \( T_c \) falling, occurs by greater reducing \( c \) parameter in contrast to the parameter \( a \). However, the linear reduction \( T_c \) calculated on equations (5) and (6) with increase \( P \) or \( x \) vastly below found in the experiment [5, 7, 10-23]. It is possible, that in this case as in the diborides with \( J < J_0 \), a reason of increasing a velocity of \( T_c \) falling is raising a loss of boron atoms by shortening \( a \) parameter with the growing of pressure or \( x \) increase.

It is shown by experiment that isovalent substitution of Mg$^{2+}$ on Zn$^{2+}$ which size is only little more (\( RSh =0.88 \AA, RP =0.74 \AA \)) than Mg (\( RSh =0.86 \AA, RP =0.65 \AA \)) can very small to rise \( T_c \) [9]. Our calculations (N 96-100) also confirm this conclusion. In work [7] it is theoretically predicted that partial substituting in MgB$_2$ of Mg$^{2+}$ on Ca$^{2+}$ or Na$^{+}$ must result in the growing \( T_c \) up to 52 K or 53 K, accordingly. Calculated by us structural parameters \( T_c \) of
these systems are close to the data of [7]: with the growing x from 0 to 0.2 $T_c^{\text{Ta.RSh}} \left( T_c^{\text{Ta.RP}} \right)$ of the systems Mg$_{1-x}$Ca$_x$B$_2$ (N 85, 89-92) and Mg$_{1-x}$Na$_x$B$_2$ (N 85, 93-95) goes up to 47 K (59 K) and 50 K (57 K), accordingly.

It follows from this that $T_c$ raising in MgB$_2$ can be reached by conservation of stoichiometry in B$_2$ plane by means of increasing the effective interplanar distances $D_1$ and $D_2$ by partial substituting Mg$^{2+}$ on the ions of greater size with charges 1+ or 2+, such as Na$^{1+}$, K$^{1+}$, Cd$^{2+}$ or Ca$^{2+}$.

It that way, the empirical dependence of $T_c(J)$ can be useful for the prognostication of the composition of new diborides with high $T_c$, and also for the estimation of $T_c$ and the correctness of determination of the structure AB$_2$ and the composition of A-cation planes. The $J$ value is not a simple ratio of geometric structural parameters of diborides. As in HTSC cuprates [27] a value of $J$ ratio depends on all these factors which influence on $T_c$ found experimentally, such as $d(B-B)$ and $d(B_2-A)$, which have an original sense and give also an information about the hole concentration, and on the size and charge of A «cations” and doping atoms too.

4. CONCLUSIONS

In our work we examined a possibility of increasing $T_c$ in AB$_2$ diborides with the structure of AlB$_2$ on the ground of empirical correlation of $T_c$ with the crystal chemical parameters of anisotropic three-dimensional fragment – A$_2$(B$_2$)–sandwich, as there is in HTSC cuprates. By this parabolic dependence, $T_c$ is correlated with the ratio ($J$) of $d(B-B)$ distances between B atoms situated at the ends of diagonal of hexagons in B$_2$ plane and sum of “effective” distances ($D_1+D_2$) from B$_2$ plane to two adjacent planes of A “cations”, taking into account by calculation a charge size of these cations and doping atoms ($J = d(B-B)/(D_1+D_2)$). We calculate the $T_c$ of diborides by this correlation (Table I). It follows:

- Among the diborides considered a superconductivity can to be only in diborides W, Mo, Ru, Os and Ta, where $J<J_0$, and Mg, Cu(II), Ag(I) and Au(I), where $J>J_0$. The result obtained there suggest that the empirical absence or low-temperature superconductivity established in transition metal diborides with $J<J_0$ might be explained of presence B vacancies in B$_2$ plane. In the absence of vacancies in B$_2$ plane $T_c$ of AB$_2$ diborides (A=W, Mo, Ru, Os) can be higher 77K, and in TaB$_2$ to reach 10K. For appearance of superconductivity and increasing
$T_c$ in NbB$_2$ and TaB$_2$ to need introduction of Nb(Ta)-vacancies or partial substitution of
Nb$^{5+}$ (Ta$^{5+}$) on Al$^{3+}$, Ti$^{4+}$ or V$^{5+}$.

- Partial substitution of W, Mo, Ru and Os on more large cations with lower charge decreases
  $T_c$ with respect to one in initial diborides, but allows to conserve a stoichiometry in B$_2$
  plane and to make a superconductors with enough high $T_c$.
- Partial substitution in MgB$_2$ of Mg on larger but with lower charge “cations” must heighten
  $T_c$.
- By the pressure $T_c$ must increase in superconductors with $J\leq J_0$ and decrease in ones with
  $J > J_0$.
- Critical crystal chemical parameters controlling $T_c$, apart from the concentration of charge
  carriers in B$_2$ plane, are the distances between boron atoms in B$_2$ plane and the parameters
  characterised the space between of B$_2$ plane and A “cation” planes in sandwich A$_2$(B$_2$), such
  as: an interval between the surface of the planes, the inhomogeneity surface of A-cation
  planes, and also the electric fields induced by the A ”cations” and doping “cations” charges.

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Fig. 1. The variation of the lattice parameters $c$ in AB$_2$ diborides as a function of Shannon crystal radii (a) and Pauling crystal ion radii (b) of A “cations”.

Fig. 2. $T_c$ as a function of $J$ in the diborides AB$_2$. $J$ was calculated by using Shannon (solid symbols -•) and Pauling (open symbols - ) radii systems: (a) $T_c^{Ta,RS}_{RS}$ ($R_{RS}$) and $T_c^{Ta,RP}_{RP}$ of Eq. 5 and Eq.6 obtained on the data for MgB$_2$, AlB$_2$ and TaB$_2$; (b) $T_c^{Zr,RS}_{RS}$ ($R_{RS}$) and $T_c^{Zr,RP}_{RP}$ of Eq. 7 and Eq.8 obtained on the data for MgB$_2$, AlB$_2$ and ZrB$_2$. 
| N | Compound               | $T_{c}^{\text{exp}}$ (K) | $a$ (Å)  | $c$ (Å)  | $D_1^R$ + $D_2^R$ | $J_{R}$ | $T_{c}^{T_{c, R}}$ (K) | $D_1^R$ + $D_2^R$ | $J_{R}$ | $T_{c}^{T_{c, R}}$ (K) | Refer. |
|---|------------------------|-------------------------|----------|----------|-------------------|--------|------------------------|-------------------|--------|------------------------|--------|
| 1.| RuB$_2$ (6+)           | -                       | 2.852    | 2.855    | -1.255            | 2.624  | 98.1                   | -                 | -      | -                      | [29]   |
| 2.| OsB$_2$ (6+)           | -                       | 2.876    | 2.871    | -1.239            | 2.680  | 97.2                   | -                 | -      | -                      | [29]   |
| 3.| MnB$_2$ (4+)           | -                       | 3.007    | 3.037    | 0.357             | 9.726  | Non-SC                 | -                 | -      | -                      | [29], [62] |
| 4.| Mn$_{0.64}$Mo$_{0.36}$B$_2$ | -                       | 3.036    | 3.098    | 0.513             | 6.828  | Non-SC                 | -                 | -      | -                      | [41]   |
| 5.| WB$_2$                 | -                       | 3.020    | 3.050    | -1.390            | 2.509  | 99.7                   | -1.030            | -3.386 | 290.0                  | [42]   |
| 6.| VB$_2$                 | -                       | 2.998    | 3.057    | -0.343            | 10.093 | Non-SC                 | 0.107             | 32.353 | Non-SC                 | [42], [61] |
| 7.| VB$_3$                 | -                       | 3.000    | 3.060    | -0.340            | 10.188 | Non-SC                 | 0.110             | 31.492 | Non-SC                 | [43]   |
| 8.| V$_{0.50}$Cr$_{0.50}$B$_2$ | -                       | 2.990    | 3.045    | -0.426            | -8.102 | Non-SC                 | 0.112             | 30.917 | Non-SC                 | [44]   |
| 9.| Cr$_2$ (3+)            | -                       | 2.969    | 3.0668   | 0.801             | 4.280  | Non-SC                 | 0.996             | 3.442  | Non-SC                 | [45]   |
| 10.| CrB$_2$ (3+)           | -                       | 2.970    | 3.070    | 0.805             | 4.260  | Non-SC                 | 1.000             | 3.429  | Non-SC                 | [29]   |
| 11.| Cr$_{0.98}$Al$_{0.02}$B$_2$ | -                       | 2.992    | 3.106    | 0.851             | 4.057  | Non-SC                 | 1.081             | 3.197  | Non-SC                 | [46]   |
| 12.| Cr$_{0.60}$Mo$_{0.40}$B$_2$ | -                       | 3.069    | 3.112    | 1.163             | 3.046  | Non-SC                 | 0.710             | 4.992  | Non-SC                 | [44]   |
| 13.| MoB$_2$                | -                       | 3.039    | 3.055    | -1.325            | -2.648 | 97.7                   | -0.665            | -5.277 | 256.2                  | [47]   |
| 14.| MoB$_2$                | -                       | 3.050    | 3.080    | -1.300            | -2.709 | 96.8                   | -0.640            | -5.503 | 247.4                  | [44]   |
| 15.| MoB$_2$                | -                       | 3.050    | 3.113    | -1.267            | -2.780 | 95.6                   | -0.607            | -5.802 | 234.2                  | [29], [48] |
| 16.| MoB$_2$                | -                       | 3.005    | 3.173    | -1.207            | -2.875 | 94.0                   | -0.547            | -6.344 | 205.7                  | [49]   |
| 17.| Mo$_{0.57}$Nb$_{0.28}$B$_2$ | -                       | 3.068    | 3.143    | -1.276            | -2.776 | 95.7                   | -0.587            | -6.039 | 222.5                  | [50]   |
| 18.| Mo$_{0.50}$Ti$_{0.50}$B$_2$ | -                       | 3.044    | 3.207    | -1.396            | -2.518 | 99.6                   | -0.593            | -5.931 | 227.9                  | [44]   |
| 19.| TiB$_2$                | -                       | 3.030    | 3.227    | 0.247             | 14.165 | Non-SC                 | 0.507             | 6.901  | Non-SC                 | [45]   |
| 20.| TiB$_2$                | -                       | 3.030    | 3.230    | 0.250             | 13.995 | Non-SC                 | 0.510             | 6.860  | Non-SC                 | [29]   |
| 21.| TiB$_2$                | -                       | 3.031    | 3.238    | 0.258             | 13.560 | Non-SC                 | 0.518             | 6.757  | Non-SC                 | [51]   |
| 22.| TiB$_2$                | -                       | 3.038    | 3.239    | 0.259             | 13.540 | Non-SC                 | 0.519             | 6.759  | Non-SC                 | [52]   |
| 23.| Ti$_{1.0}$Cr$_{0.50}$B$_2$ | -                       | 2.990    | 3.140    | 0.182             | 19.000 | Non-SC                 | 0.477             | 7.239  | Non-SC                 | [44]   |
| 24.| CuB$_2$ (2+)           | -                       | 2.960    | 3.250    | 1.510             | 2.263  | 26.0                   | 1.870             | 1.828  | 15.3                   | [53]   |
| 25.| AgB$_2$ (3+)           | -                       | 3.000    | 3.240    | 0.570             | 6.077  | Non-SC                 | -                 | -      | Non-SC                 | [29]   |
| N  | Compound          | $T_c^{\text{exp}}$ (K) | $a$ (Å)  | $c$ (Å)  | $D_1^{\text{Rh}} + D_2^{\text{Rh}}$ | $J_{\text{Rh}}^{\text{Rh}}$ (K) | $T_c^{\text{Ta,Rh}}$ (K) | $D_1^{\text{Rh}} + D_2^{\text{Rh}}$ | $J_{\text{RP}}$ | $T_c^{\text{Ta,RP}}$ (K) | Refer. |
|----|-------------------|------------------------|----------|----------|-------------------------------------|-------------------------------|-------------------------------|-------------------------------------|-------------|----------------------------|--------|
| 26.| AgB$_2$ (1+)      | 59*                    | 2.980*   | 3.920*   | 2.630                               | 1.308                        | 62.8                         | 2.660                               | 1.294       | 68.3                      | [53]   |
| 27.| TaB$_2$           | 9.5                    | 3.082    | 3.243    | -0.657                              | -5.417                       | 9.5                          | -0.407                              | -8.744      | 9.5                       | [37]   |
| 28.| TaB$_2$ Non-SC    | -                      | 3.087    | 3.247    | -0.6538                             | -5.459                       | 7.4                          | -0.403                              | -8.845      | Non-SC                    | [39]   |
| 29.| TaB$_2$           | -                      | 3.080    | 3.270    | -0.630                              | -5.645                       | Non-SC                       | -0.380                              | -9.359      | Non-SC                    | [29], [44]|
| 30.| TaB$_2$ -          | -                      | 3.065    | 3.283    | -0.617                              | -5.736                       | Non-SC                       | -0.367                              | -9.643      | Non-SC                    | [54]   |
| 31.| Ta$_{0.50}$V$_{0.50}$B$_2$ | - | 3.040 | 3.160 | -0.791 | -4.450 | 50.8 | -0.542 | -6.476 | 197.9 | [55] |
| 32.| Ta$_{0.50}$Cr$_{0.50}$B$_2$ | - | 3.025 | 3.210 | -0.873 | -4.000 | 66.2 | -0.561 | -6.220 | 212.7 | [44] |
| 33.| Ta$_{0.50}$Ti$_{0.50}$B$_2$ | - | 3.050 | 3.246 | -0.741 | -4.750 | 39.2 | -0.463 | -7.607 | 116.7 | [44] |
| 34.| Ta$_{0.77}$Al$_{0.23}$B$_2$ | - | 3.060 | 3.294 | -0.681 | -5.185 | 20.4 | -0.412 | -8.580 | 26.6 | [56] |
| 35.| NbB$_2$ Non-SC    | -                      | 3.110    | 3.370    | -0.566                              | -6.341                       | Non-SC                       | -0.297                              | -12.105     | Non-SC                    | [55]   |
| 36.| Nb$_{0.50}$Hf$_{0.50}$B$_2$ | - | 3.120 | 3.400 | -0.531 | -6.780 | Non-SC | -0.266 | -12.762 | Non-SC | [44] |
| 37.| AlB$_2$            | -                      | 3.005    | 3.257    | 1.232                               | 2.816                        | Non-SC                       | 1.757                               | 1.975       | Non-SC                    | [40]   |
| 38.| AlB$_2$ Non-SC    | -                      | 3.009    | 3.262    | 1.237                               | 2.809                        | 0                           | 1.762                               | 1.972       | 0                         | [29], [57]|
| 39.| NbB$_2$ -          | -                      | 3.110    | 3.267    | -0.633                              | -5.673                       | Non-SC                       | -0.233                              | -15.412     | Non-SC                    | [39]   |
| 40.| NbB$_2$ -          | -                      | 3.090    | 3.300    | -0.600                              | -5.947                       | Non-SC                       | -0.200                              | -17.840     | Non-SC                    | [29]   |
| 41.| Nb$_{0.67}$Al$_{0.33}$B$_2$ | - | 3.068 | 3.334 | -0.673 | -5.267 | 16.7 | -0.205 | -17.319 | Non-SC | [56] |
| 42.| Nb$_{0.50}$V$_{0.50}$B$_2$ | - | 3.030 | 3.200 | -0.748 | -4.678 | 42.1 | -0.326 | -10.747 | Non-SC | [55] |
| 43.| Nb$_{0.50}$Zr$_{0.50}$B$_2$ | - | 3.128 | 3.420 | 0.510 | -7.081 | Non-SC | -0.084 | -43.220 | Non-SC | [44] |
| 44.| HfB$_2$            | -                      | 3.140    | 3.470    | 0.070                               | 51.797                       | Non-SC                       | 0.230                               | 15.764      | Non-SC                    | [29]   |
| 45.| HfB$_2$ -          | -                      | 3.141    | 3.470    | 0.070                               | 51.813                       | Non-SC                       | 0.230                               | 15.769      | Non-SC                    | [42], [44]|
| 46.| HfB$_2$            | -                      | 3.139    | 3.473    | 0.073                               | 49.650                       | Non-SC                       | 0.233                               | 15.588      | Non-SC                    | [58]   |
| 47.| Hf$_{0.50}$Ti$_{0.50}$B$_2$ | - | 3.085 | 3.368 | -0.034 | -104.4 | Non-SC | 0.139 | 25.595 | Non-SC | [44] |
| 48.| AuB$_2$ (3+)       | -                      | 3.140    | 3.510    | 0.540                               | 6.714                        | Non-SC                       | -                                   | -           | -                         | [29]   |
| 49.| AuB$_2$ (1+)       | 72*                    | 2.980*   | 4.050*   | 2.540                               | 1.355                        | 61.3                         | 2.680                               | 1.284       | 69.2                      | [53]   |
| 50.| ScB$_2$            | -                      | 3.146    | 3.517    | 0.863                               | 4.209                        | Non-SC                       | 1.087                               | 3.342       | Non-SC                    | [29]   |
| 51.| MgB$_2$            | 49.0                   | 3.068    | 3.505    | 1.785                               | 1.985                        | 37.8                         | 2.205                               | 1.607       | 37.9                      | [31]   |
| N | Compound | $T_c^{exp}$ (K) | $a$ (Å) | $c$ (Å) | $D_1^{RSh} + D_2^{RSh}$ | $J_{RSh}$ | $T_c^{Ta,RSh}$ (K) | $D_1^{RP} + D_2^{RP}$ | $J_{RP}$ | $T_c^{Ta,RP}$ (K) | Refer. |
|---|----------|----------------|--------|--------|------------------------|---------|-------------------|------------------------|---------|-------------------|--------|
| 52. | MgB$_2$ | 36.6 | 3.075 | 3.519 | 1.799 | 1.974 | 38.3 | 2.219 | 1.600 | 38.6 | [32] |
| 53. | MgB$_2$ | 39.0 | 3.0856 | 3.5199 | 1.800 | 1.979 | 38.1 | 2.220 | 1.605 | 38.1 | [33] |
| 54. | MgB$_2$ | 38.8 | 3.083 | 3.520 | 1.800 | 1.978 | 38.1 | 2.220 | 1.604 | 38.2 | [34] |
| 55. | MgB$_2$ | - | 3.085 | 3.520 | 1.800 | 1.979 | 38.1 | 2.220 | 1.605 | 38.1 | [7] |
| 56. | MgB$_2$ | 38.1 | 3.0851 | 3.5201 | 1.801 | 1.978 | 38.1 | 2.221 | 1.604 | 38.2 | [36] |
| 57. | MgB$_2$ | 39.0 | 3.0849 | 3.5211 | 1.801 | 1.978 | 38.1 | 2.221 | 1.604 | 38.2 | [35] |
| 58. | MgB$_2$ | 38.9 | 3.0846 | 3.5230 | 1.803 | 1.975 | 38.3 | 2.223 | 1.602 | 38.4 | [5] |
| 59. | MgB$_2$ | 39.0 | 3.086 | 3.524 | 1.804 | 1.975 | 38.3 | 2.224 | 1.602 | 38.3 | [1] |
| 60. | ZrB$_2$ | - | 3.169 | 3.523 | 0.083 | 44.084 | Non-SC | 0.323 | 11.328 | Non-SC | [59] |
| 61. | ZrB$_2$ | - | 3.150 | 3.530 | 0.090 | 40.415 | Non-SC | 0.330 | 11.022 | Non-SC | [29] |
| 62. | ZrB$_2$ | 5.5 | 3.170 | 3.532 | 0.092 | 39.787 | Non-SC | 0.332 | 11.025 | Non-SC | [39] |
| 63. | ZrB$_2$ | - | 3.166 | 3.535 | 0.095 | 38.482 | Non-SC | 0.335 | 10.913 | Non-SC | [45] |
| 64. | Zr$_{0.50}$Ti$_{0.50}$B$_2$ | - | 3.098 | 3.390 | -0.054 | -66.76 | Non-SC | 0.205 | 17.414 | Non-SC | [44] |
| 65. | LuB$_2$ | - | 3.246 | 3.704 | 0.702 | 5.339 | Non-SC | 0.914 | 4.101 | Non-SC | [42] |
| 66. | YB$_2$ | - | 3.290 | 3.835 | 0.715 | 5.313 | Non-SC | 1.045 | 3.635 | Non-SC | [60] |
| 67. | PuB$_2$ (4+) | - | 3.180 | 3.900 | -0.100 | -36.72 | Non-SC | - | - | - | [29] |
| 68. | UB$_2$ (4+) | - | 3.136 | 3.988 | -0.132 | 27.433 | Non-SC | 0.108 | 33.529 | Non-SC | [42] |
| 69. | UB$_2$ (4+) | - | 3.140 | 4.000 | -0.120 | 30.215 | Non-SC | 0.120 | 30.215 | Non-SC | [29] |
| 70. | MgB$_2$ | 38.2 | 3.0859 | 3.5212 | 1.801 | 1.978 | 38.1 | 2.221 | 1.604 | 38.2 | [17] |
| 71. | MgB$_2$, 1.17 GPa | - | 3.0802 | 3.5112 | 1.791 | 1.986 | 37.8 | 2.211 | 1.608 | 37.8 | [17] |
| 72. | MgB$_2$, 2.14 GPa | - | 3.0715 | 3.4985 | 1.778 | 1.994 | 37.5 | 2.198 | 1.613 | 37.3 | [17] |
| 73. | MgB$_2$, 3.05 GPa | - | 3.0671 | 3.4885 | 1.768 | 2.002 | 37.2 | 2.188 | 1.618 | 36.7 | [17] |
| 74. | MgB$_2$, 4.07 GPa | - | 3.0635 | 3.4819 | 1.762 | 2.008 | 36.9 | 2.182 | 1.621 | 36.4 | [17] |
| 75. | MgB$_2$, 5.09 GPa | - | 3.0545 | 3.4718 | 1.752 | 2.013 | 36.7 | 2.172 | 1.624 | 36.1 | [17] |
| 76. | MgB$_2$, 6.53 GPa | - | 3.0497 | 3.4586 | 1.739 | 2.025 | 36.2 | 2.159 | 1.631 | 35.4 | [17] |
| 77. | MgB$_2$, 8.02 GPa | - | 3.0484 | 3.4572 | 1.737 | 2.026 | 36.2 | 2.157 | 1.632 | 35.3 | [17] |
# TABLE I. (cont.)

| N | Compound | $T_c^{\text{exp}}$ (K) | $a$ (Å) | $c$ (Å) | $D_1^{RSh} + D_2^{RSh}$ | $J_{RSh}$ | $T_c^{Ta,RSh}$ (K) | $D_1^{RP} + D_2^{RP}$ | $J_{RP}$ | $T_c^{Ta,RP}$ (K) | Refer. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 78. | MgB$_2$ | - | 3.0906 | 3.5287 | 1.809 | 1.973 | 38.3 | 2.229 | 1.601 | 38.5 | [18] |
| 79. | MgB$_2$, 6.15 GPa | - | 3.0646 | 3.4860 | 1.766 | 2.004 | 37.1 | 2.186 | 1.619 | 36.6 | [18] |
| 80. | MgB$_2$ | - | 3.085 | 3.523 | 1.803 | 1.976 | 38.2 | 2.223 | 1.602 | 38.4 | [40] |
| 81. | Al$_{0.39}$Mg$_{0.61}$B$_2$ | - | 3.047 | 3.369 | 1.763 | 1.996 | 37.4 | 2.193 | 1.604 | 38.1 | [40] |
| 82. | Al$_{0.50}$Mg$_{0.50}$B$_2$ | - | 3.047 | 3.366 | 1.450 | 2.426 | 18.6 | 2.000 | 1.759 | 22.4 | [40] |
| 83. | Al$_{0.67}$Mg$_{0.33}$B$_2$ | - | 3.037 | 3.331 | 1.374 | 2.552 | 12.8 | 1.915 | 1.831 | 14.9 | [40] |
| 84. | Al$_{0.75}$Mg$_{0.25}$B$_2$ | - | 3.030 | 3.302 | 1.327 | 2.637 | 8.6 | 1.864 | 1.877 | 10.1 | [40] |
| 85. | MgB$_3$ | - | 3.065 | 3.5186 | 1.799 | 1.968 | 38.5 | 2.219 | 1.595 | 39.1 | [7] |
| 86. | Mg$_{0.98}$Al$_{0.02}$B$_2$ | - | 3.084 | 3.5158 | 1.802 | 1.976 | 38.2 | 2.223 | 1.602 | 38.4 | [7] |
| 87. | Mg$_{0.96}$Al$_{0.04}$B$_2$ | - | 3.083 | 3.5115 | 1.804 | 1.974 | 38.3 | 2.225 | 1.600 | 38.6 | [7] |
| 88. | Mg$_{0.92}$Al$_{0.08}$B$_2$ | - | 3.081 | 3.4969 | 1.802 | 1.974 | 38.3 | 2.224 | 1.600 | 38.6 | [7] |
| 89. | Mg$_{0.95}$Ca$_{0.05}$B$_2$ | - | 3.072* | 3.5451* | 1.855 | 1.912 | 40.8 | 2.304 | 1.541 | 44.4 | [7] |
| 90. | Mg$_{0.90}$Ca$_{0.10}$B$_2$ | - | 3.080* | 3.5728* | 1.913 | 1.859 | 42.9 | 2.392 | 1.487 | 49.7 | [7] |
| 91. | Mg$_{0.85}$Ca$_{0.15}$B$_2$ | - | 3.087* | 3.6025* | 1.974 | 1.805 | 45.0 | 2.483 | 1.435 | 54.8 | [7] |
| 92. | Mg$_{0.80}$Ca$_{0.20}$B$_2$ | 52* | 3.095* | 3.6304* | 2.035 | 1.756 | 46.9 | 2.574 | 1.388 | 59.3 | [7] |
| 93. | Mg$_{0.95}$Na$_{0.05}$B$_2$ | - | 3.063* | 3.5592* | 1.870 | 1.892 | 41.6 | 2.288 | 1.546 | 43.9 | [7] |
| 94. | Mg$_{0.90}$Na$_{0.10}$B$_2$ | - | 3.061* | 3.5967* | 1.940 | 1.822 | 44.4 | 2.356 | 1.500 | 48.4 | [7] |
| 95. | Mg$_{0.80}$Na$_{0.20}$B$_2$ | 53* | 3.057* | 3.6776* | 2.094 | 1.686 | 49.6 | 2.505 | 1.409 | 57.3 | [7] |
| 96. | MgB$_2$ | 38.5 | 3.0787 | 3.5178 | 1.798 | 1.977 | 38.2 | 2.218 | 1.603 | 38.3 | [8] |
| 97. | Mg$_{0.97}$Zn$_{0.03}$B$_2$ | 38.4 | 3.0870 | 3.5241 | 1.805 | 1.974 | 38.3 | 2.233 | 1.596 | 38.9 | [9] |
| 98. | Mg$_{0.95}$Zn$_{0.05}$B$_2$ | 38 | 3.0803 | 3.5226 | 1.805 | 1.972 | 38.4 | 2.238 | 1.589 | 39.7 | [8] |
| 99. | Mg$_{0.90}$Zn$_{0.10}$B$_2$ | 38.3 | 3.0841 | 3.5250 | 1.809 | 1.968 | 38.5 | 2.256 | 1.579 | 40.6 | [8] |
| 100. | Mg$_{0.80}$Zn$_{0.20}$B$_2$ | 38.3 | 3.0841 | 3.5239 | 1.812 | 1.965 | 38.7 | 2.285 | 1.558 | 42.7 | [8] |

* - $T_c$ and lattice constant are calculated.