Crimson Publishers
Wings to the Research

Mini Review

Recent Trend on Superconductivity of Two-Dimensional Magnesium Boride

Qida Dun and Xin Qu*

Key Laboratory of Functional Materials Physics and Chemistry of the Ministry of Education, Key Laboratory of Functional Materials Physics and Chemistry of the Ministry of Education, College of Physics, Jilin Normal University, Changchun 130103, China

ISSN : 2688-8394

Abstract

Research on two-dimensional superconducting materials has become a hot topic in the field of scientific research in recent years. The main objective of research on superconducting materials is to obtain materials with high transition temperature(Tc), while ensuring their reliable stability and appropriate cost. Two-dimensional magnesium borides, as the most outstanding among two-dimensional metal borides, have been studied by many scholars in recent years. This paper will focus on describing the study trend of magnesium borides in recent years.

Keywords: Superconductivity; Two-Dimensional magnesium boride; Density functional theory

***Corresponding author:** Xin Qu, Key Laboratory of Functional Materials Physics and Chemistry of the Ministry of Education, Key Laboratory of Functional Materials Physics and Chemistry of the Ministry of Education, College of Physics, Jilin Normal University, Changchun 130103, China

Submission: March 05, 2023
Published: March 13, 2023

Volume 3 - Issue 5

How to cite this article: Qida Dun and Xin Qu*. Recent Trend on Superconductivity of Two-Dimensional Magnesium Boride. Ann Chem Sci Res. 3(5). ACSR. 000571. 2023. DOI: 10.31031/ACSR.2023.03.000571

Mini Review

The bulk MgB_2 synthesized in the laboratory in 2000 has caused great influence in the field of materials. According to the experimental and theoretical calculation, its transition temperature is as high as 39K. Due to its suitable cost and high transition temperature, these characteristics have brought new research ideas for the research of superconducting materials at that time. In order to further understand the superconducting mechanism of bulk MgB_2, Kortus et al. [1] calculated the energy band structure in 2001 and drew the following conclusions: Mg is ionized in bulk MgB_2 and this compound is produced by the combination of covalent B-B andionic B-Mg bonds. Its own properties and structure indicate that it is a typical *sp* metal. Strong electron-ion scattering is caused by strong bond and strong electron-phonon coupling is generated to produce strong superconductivity [1]. The discovery of graphene in 2004 pioneered two-dimensional materials and its excellent properties have led many scholars to continuously study two-dimensional materials. The superconductivity of two-dimensional metal borides has become a research hotspot in recent years, among which the superconductivity of two-dimensional metal borides MgB_2 is the most studied two-dimensional metal borides. The following figure shows the transition temperatures of the materials involved in the article (Table 1).

Table 1: Transition temperatures of the magnesium boride materials.

Materials	Transition Temperature
Bulk MgB_2	39K
MgB_4	52K
B_2MgB_2	23.2K
B_4MgB_4	13.3K
Partial bulk Mg-B system	<3K
$Mg_{0.5}Ba_{0.5}B_2$	63.6 ± 6.6K
Single layer MgB_2 under hydrogen atoms	67K
MgB_2/Graphene double layer film	36K

At present, due to the progress of science and technology, the exploration of material properties has more advanced technology in calculation and observation, thus producing less error, which also has a deeper understanding of the superconducting mechanism of MgB_2. Guerfi [2] used density functional theory (DFT) to further explore MgB_2 superconductivity

in the generalized gradient approximation (GGA) pseudo-potential and plane-wave-based method, as well as the frozen phonon method and discovered that the superposition of the A_{2u} and the E_{2g} vibration mode is a key factor in the superconducting mechanism of MgB_2 [2]. Superconducting gap is one of the important indexes to evaluate the properties of superconducting materials. The familiar bulk MgB_2 has two superconducting gaps. When the thickness of MgB_2 is small and reaches the limit state (about the thickness of atomic layer), the relevant properties can be predicted through the first principles calculation and the theoretical calculation of Eliasberg equation. In the vertical direction of quantum constraint, the sub-bands in the superconducting film are usually separated, because the separation of sub-bands will generate more superconducting gaps in the superconducting material. Resulting in multiple bands and possibly multi-gap superconductivity. With the emerging surface contribution, a single layer of MgB_2 produces three distinct superconducting gaps in the completely separated portion of the Fermi surface and a three-layer superconducting gap superconductor is predicted. Until now, the known effects of multi-gap superconductors include vortex and electronic states, giant paramagnetic response, hidden criticality and time-reversed symmetry breaking, etc. [3]. However, in order to better understand the above properties of multi-gap superconductors, there is still a lack of more materials to systematically study the current situation. There is also a very special connection between two-dimensional materials and multi-gap superconductors, one that has not been explored until now: "Surface states can equally accommodate new superconducting gaps." The study of Mg-B superconducting gap does not stop there. Currently, it is predicted that MgB_4 of three thin films can excite four gap superconducting properties at a higher transition temperature than traditional Mg borides, ranging from Tc to 52K [4]. Although the results are predicted, they also provide new ideas for the development of superconducting materials in the future. The theoretical prediction proves that the Fermi surface is closely related to its high Tc four-gap superconductivity. The Fermi surface exhibits unusually strong electron-phonon coupling and has obvious four-region distribution characteristics.

Although the bulk MgB_2 exhibits high transition temperatures, not all Mg borides have high transition temperatures. Using first-principles calculations, Xiao Bao Yang et al. [5] studied the structure, electronic and superconducting properties of Mg intercalated bilayer borene BxMgBx (x=2-5).Among all the studied materials, B_2MgB_2 and B_4MgB_4 show the highest phonon-mediated superconductivity with high transition temperatures (Tc) of 23.2K and 13.3K, respectively, although their transition temperatures are much lower than those of 39K.In other bulk Mg-B systems, the transition temperature Tc is estimated to be lower than 3 K. The calculated Tc of two-dimensional B_2MgB_2 calculated from the layered MgB_2 is 23.2K, which is the highest Tc in the low-dimensional Mg-B system [5].

Two-dimensional materials have always been regarded as the most promising materials. Compared with bulk magnesium boride, the large difference in transition temperature between two-dimensional magnesium boride and bulk magnesium boride is a point worth paying attention to. How to improve the transition temperature of two-dimensional magnesium boride determines whether it can be applied more widely.

In recent years, the main research direction of magnesium boride is how to increase its transition temperature. The commonly used methods to increase the transition temperature include electron doping and biaxial strain [6-9]. The influence of the former on the transition temperature is discussed first. Electron doping: Doping atoms different from Mg into MgB_2 to obtain $Mg_{1-x}M_xB_2$. Here, we discuss the related properties of the compounds obtained by doping different kinds of atoms into MgB_2.

Ian Mackinnon et al. [8] doped Sc, Ti, Cd, Ba and Al to obtain $Mg_{1-x}M_xB_2$. In terms of the prediction of transition temperature, they used the DFT calculation and found that the change of phonon dispersion diagram changes with the doping of electrons. Interestingly, the substitution of Mg in electron doping may lead to the inhibition of Tc. We know that phonon-electron coupling is one of the factors affecting the transition temperature and that electron doping can lead to phonon and electron-phonon renormalization, thus changing the transition temperature. However, it is not the case that the more doped atoms will have a greater effect on the transition temperature. The two are not simple linear relationship, $Mg_{1-x}M_xB_2$, for example experimental and computational predictions show that adding 25% Al to MgB_2 results in phonon and electron-phonon renormalization which makes phonon frequency renormalization strongest. As mentioned above, electron doping may lead to Tc inhibition, but it also has an effect on the increase of transition temperature. By doping Ba into MgB≠, the transition temperature of $Mg_{0.5}Ba_{0.5}B_2$ can be predicted as high as 63.6±6.6K by theoretical calculation. This is also the highest predicted transition temperature of $Mg_{1-x}M_xB_2$ at present. Therefore, Jose A Alarco et al. [7] have new expectations for BaB_2. The Tc of BaB_2 predicted by theoretical calculation is significantly higher than that of other diborides at present, but its structure is not stable. In order to stabilize its structure, 16GPa should be applied to stabilize the structure.

The effect of biaxial strain on the transition temperature is much more obvious than that of electron doping. Zhao Liu et al. [9] studied the effect of biaxial strain on the superconducting properties of MgB_2 monomolecular layer by using the first-principles calculation method. By applying different degrees of biaxial strain to the material, the team conducted phonon dispersion analysis and obtained relevant experimental data to determine the phonon dispersion stability. The experimental data show that a biaxial strain of 7% can be applied to MgB_2 without generating any imaginary frequency. While the calculation of the material transition temperature still needs to be judged by theoretical calculation, the team calculated the two-gap superconductivity of MgB_2 based on the superconducting properties of the Migdal-Eliasberg theoretical framework. The data show that the critical temperature of MgB_2 is increased by ~20% when the tensile biaxial strain is applied to the material, while the compressive biaxial strain can reduce the critical temperature of MgB_2 by ~29%.Compared with electron doping, biaxial strain is often easier to experiment.

Both electron doping and biaxial strain can affect the superconducting transition temperature of materials, and different ways can lead to the increase and suppression of the transition temperature. After referring to more literature materials, it is found that the main way for most materials to raise the transition temperature is biaxial strain, which has a great influence on the transition temperature and can better control the rise and fall of the transition temperature. In addition to these two main methods, there are some other methods that can have a great impact on the transition temperature of magnesium boride.

As for the method of changing the transition temperature, the influence of hydrogen atoms on the superconducting properties of monolayer MgB_2 has also been studied, Bekaert et al. [10] by solving the Eliaschberg equation for complete anisotropy, combined with first-principles descriptions of electronic state and vibrational dynamics and the coupling between them. The results show that the critical temperature caused by hydrogenation is 67K and the biaxial tensile strain can increase it to more than 100K, which also indicates that if various ways of changing the transformation temperature can be combined, it may lead to breakthrough discoveries on the transformation temperature raising of superconducting materials.

Two-dimensional metal borides not only have good superconductivity, but also show good application in combination with other materials. Studies have shown that graphene itself lacks superconductivity and MgB_2/graphene bilayer films obtained by combining MgB_2 with graphene can induce the superconductivity of graphene through the proximity effect [11]. In terms of synthesis, a single layer of graphene grown on copper foil is transferred to the target substrate and then MgB_2 films are deposited on the transferred graphene using a hybrid physico-chemical vapor deposition technique. MgB_2 films obtained on graphene show a continuous film surface in the direction of the C-axis, exhibiting a narrow superconducting transition temperature Tc at 36K, which is close to the 39K transition temperature of the bulk MgB_2.

From an application point of view, the realization of magnesium boride/graphene complexes is also very attractive in terms of developing related devices that operate at high temperatures, thereby reducing low temperature costs and requirements. On various applications, with regard to MgB_2, a great deal of effort has been put into making superconducting devices or circuits in order to take advantage of its high transition temperature. In this regard, magnesium boride/graphene complexes will provide a new approach.

With the continuous development of science and technology, the requirements of materials are constantly getting higher. How to improve the superconducting performance of materials and how to improve the transition temperature of materials are the problems that need to be solved in the field of superconductivity. This paper focuses on the related superconducting properties and applications of two-dimensional magnesium boride as superconducting materials, as well as two main methods to change its transition temperature. As two-dimensional superconducting material, two-dimensional magnesium boride has the remarkable characteristic that it is a multi-gap superconductor. This multi-gap superconductivity can lead to many properties of MgB_2 that are significantly different from those of traditional single-gap superconductors. Moreover, there are new physical phenomena that do not exist in single-gap superconductors. If MgB_2 can be combined with more materials in the future, there will be more excellent properties waiting to be discovered. Electron doping and biaxial strain can effectively change the transition temperature of superconducting materials. If the application ability of these two technologies can be improved, the transition temperature of superconducting materials can be changed to the maximum extent. In a word, two-dimensional magnesium boride is the most superconducting material with excellent superconducting properties. We believe that in the future material field, it can better show its advantages as a superconducting material.

Acknowledgments

The presented study was performed with the financial support of the Program for the National Natural Science Foundation of China (Grants No. 12204194), the Program for the Development of Science and Technology of Jilin Province (Grants No. YDZJ202101ZYTS065).

References

1. Kortus J, Mazin II, Belashchenko KD, Antropov VP, Boyer LL (2001) Superconductivity of metallic boron in MgB_2. Phys Rev Lett 86: 4656-4659.
2. Geuerfi T (2020) Out-of-plane ionicity versus in-plane covalency interplay and electron--phonon coupling in MgB_2 superconductor. Chinese Journal of Physics 64: 287-294.
3. Bekaert J, Aperis A, Partoens B, Oppeneer PM, Milošević MV (2017) Evolution of multigap superconductivity in the atomically thin limit: Strain-enhanced three-gap superconductivity in monolayer MgB_2. Phys Rev B 96: 094510.
4. Yinchang Zhao, Chao Lian, Shuming Zeng, Zhenhong Dai, Sheng Meng, et al. (2020) MgB_4 trilayer film: A four-gap superconductor. Physical Review B 101: 104507.
5. Ji-Hai Liao, Yin-Chang Zhao, Yu-Jun Zhao, Hu Xu, Xiao-Bao Yang (2017) Phonon-mediated superconductivity in Mg intercalated bilayer borophenes. Physical Chemistry Chemical Physics 19(43): 29237-29243.
6. Cai Cheng, Man-Yi Duan, Zhao Wang, Xiao-Lin Zhou (2020) AlB_2 and MgB_2: A comparative study of their electronic, phonon and superconductivity properties via first principles. Philosophical Magazine 100(17).
7. Jose A Alarco, Peter C Talbot, Ian DR Mackinnon (2015) Phonon anomalies predict superconducting Tc for AlB_2-type structures. Phys Chem Chem Phys 17(38): 25090-25099.
8. Ian DR Mackinnon, Peter C Bot, Jose A Alarco (2017) Phonon dispersion anomalies and superconductivity in metal Substituted MgB_2. Computational Materials Science 130: 191-203.
9. Zhao Liu, Biao Wang (2022) Biaxial strain engineering on the superconducting properties of MgB_2 monolayer. Materials Chemistry and Physics 290: 126637.
10. Bekaert J, Petrov M, Peris A, Oppeneer PM, Milosevic MV (2019) Hydrogen-induced high-temperature superconductivity in two-dimensional materials: Example of hydrogenated monolayer MgB_2. Physical Review Letters 123: 077001.
11. Shu-Han Cheng, Yan Zhang, Hong-Zhang Wang, Yu-Long Li, Can Yang, et al. (2018) Fabrication and characterization of superconducting MgB_2 thin film on graphene. AIP Advances 8(7): 075015.

