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Research on Metal-based High-temperature Superconductors and BCS Mechanism

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Abstract. Recently, high-temperature superconductors have had a wide range of applications in fields such as electric power transportation, medical imaging and diagnostics, electronic devices, and quantum computing. Therefore, this paper reviews the properties and mechanisms of copper-oxide, iron-based, nickel-based and hydrogen-based high-temperature superconductors. The results show that optimizing the copper-oxygen layer structure and regulating the interlayer coupling are effective methods to improve the performance of copper oxide high-temperature superconductors. This method can enhance the superconducting current, thus improving their superconducting properties. For iron-based high-temperature superconductors, the superconducting transition temperature and energy gap can be enhanced by doping rare earth elements or transition metal elements, and adjusting the topology of the Fermi surface to change the internal electronic structure of the material. The double-layer structure of nickel-based high-temperature superconductors is investigated by using tensor networks and other methods, which significantly increase the Tc of the material and solve the problems of difficult preparation by detecting the impurity effect and vortex state of the material. For hydrogen-based superconductors, chemical pre-pressurization and doping with alkali metal elements are mainly used to synthesize ternary hydrogen-based superconductors and hydrogen-minor superconductors. This can significantly increase the transition temperature of superconducting materials and reduces the pressure required for their preparation. Therefore, this study can improve the superconducting properties of these high-temperature superconductors and extend their applications in the fields of electric power transportation, medical imaging and diagnostics, electronic devices and quantum computing.

Keywords: HTSCs; FeSCs; Hydrogen-based superconductors; Nickel-based superconductors.

1. Introduction

Nowadays, the characteristics of high-temperature superconducting materials, are high critical transition temperature, zero resistance phenomenon, and antimagnetism. They can make high-temperature superconducting materials widely used in low-loss electric power transport, simplified medical imaging instruments, and energy storage of new energy vehicles. It can make use of its own characteristics to improve the efficiency of power transport and facilitate the engine of medical imaging instruments and new energy vehicles and power storage devices based on RT superconductor technology.

High-temperature superconductor normally exhibit no resistance at all to conduct electricity while repelling internal electric fields when the temperature is above 77K. They are mainly suitable for the modified BCS (Bardeen-Cooper-Schrieffer) mechanism, and they focuses on electron-electron interactions. The main categories of high-temperature superconductors are metallic superconducting materials and non-metallic high-temperature superconducting materials. Copper oxide high-temperature superconductors contain the elements copper and oxygen and have a layered crystal

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structure reflecting anisotropy. Iron-based high-temperature superconductors are high-temperature superconducting materials, and their main component is iron, and usually have a complex electronic structure including multiple Fermi planes and electronic bands. Nickel-based high-temperature superconductors also have a multi-band electronic structure and are doped with different elements to regulate the electronic structure. The research of hydrogen-based high-temperature superconductors focuses on achieving high-temperature superconductivity at lower pressures or temperatures by combining other elements or compounds with the special properties of the element hydrogen. However, high-temperature superconducting materials still limit the application of these high-temperature superconducting materials due to disadvantages such as the difficulty of preparation, the lack of clarity of the basic principles of material superconductivity and the difficulty of optimising the superconducting properties of materials. Therefore, improving the properties of high-temperature superconducting materials is of great significance for expanding the applications of superconducting materials in the fields of electric power transmission, medical imaging and diagnosis, and quantum computation, as well as for the study of the fundamental principles of superconductivity.

Therefore, this paper reviews the properties and mechanisms of copper oxide, iron-based high-temperature superconductors, nickel-based high-temperature superconductors and hydrogen-based high-temperature superconductors. The results show that effective methods include optimising the copper-oxygen layer structure and modulating the interlayer coupling, which can enhance the superconducting current and optimise the superconducting properties of the materials, and thus improving the performance of copper oxide high-temperature superconductors. The electronic structure of iron-based high-temperature superconductors can be altered by doping with rare earth elements, transition metal elements, and adjusting the topology of the Fermi surface. They can significantly increase the superconducting transition temperature and energy gap of iron-based high-temperature superconducting materials. Nickel-based high-temperature superconductors can use the tensor network research method to detect the impurity effect and vortex state of the material, which can enhance the T_c of the material and solve the problem of difficult to prepare the material. The synthesis of ternary hydrogen-based superconductors and hydrogen-poor superconductors by chemical pre-pressurisation and doping with alkali metal elements is considered to be an effective method to increase the transition temperature of hydrogen-based high-temperature superconductors and to reduce the pressure required for their preparation.

2. Copper Oxide High-temperature Superconductors

Copper oxide high-temperature superconductors (HTSCs) are extensively used in superconductivity. The d-wave symmetry pairing in CuO_2 planes is the key to their superconductivity. HTSCs are favored for their high critical temperatures, strong electron correlation, and low melting points, which reduce the costs associated with cooling. Despite these benefits, HTSCs face challenges. Their brittleness makes them difficult to work with. Additionally, they are sensitive to magnetic fields, which restricts their performance and stability.

Yijun Yu et al. used the TSMG (Traveling Solvent Floating Zone Growth) melt growth technique to prepare single-layer Bi-2212 superconducting samples, as shown in Figure 1(a). It structurally has two CuO_2 planes that make up half of the unit cell structure. It exhibits a superconducting transition temperature similar to that of the bulk material, indicating that the single-layer Bi-2212 sample maintains high-temperature superconducting performance similar to three-dimensional bulk material. Liguo Ma et al. used STM (Scanning Tunneling Microscopy) technology to study its electronic structure. The spatially averaged differential conductance spectrum of STM revealed the superconducting gap and a significant coherent peak, which are very close to the gap size of the bulk material. In addition, temperature-dependent STM studies shown in Figure 1(b) further confirmed that the single-layer Bi-2212 sample has various superconducting phase characteristics identical to the bulk material, including high-temperature superconductivity, pseudogap, and charge orderliness [1]. Wu et al. prepared $Hg_2Ba_2Ca_2Cu_3O_{10+\delta}$ with a maximum T_c of about 135 K through a sealed reaction system and sintering process. Figure 1(c) shows the crystal structures of three Hg-cuprate

superconductors, with the oxygen sites of the Hg layer being partially occupied. The 1201 structure has apical oxygen atoms above and below the Cu site, while the inner CuO_2 layer of the 1223 structure lacks apical oxygen atoms. These materials can exhibit excellent superconducting properties due to their structural differences, and superconducting properties can be due to different interaction levels caused by different electronic doping levels of the CuO_2 layers.

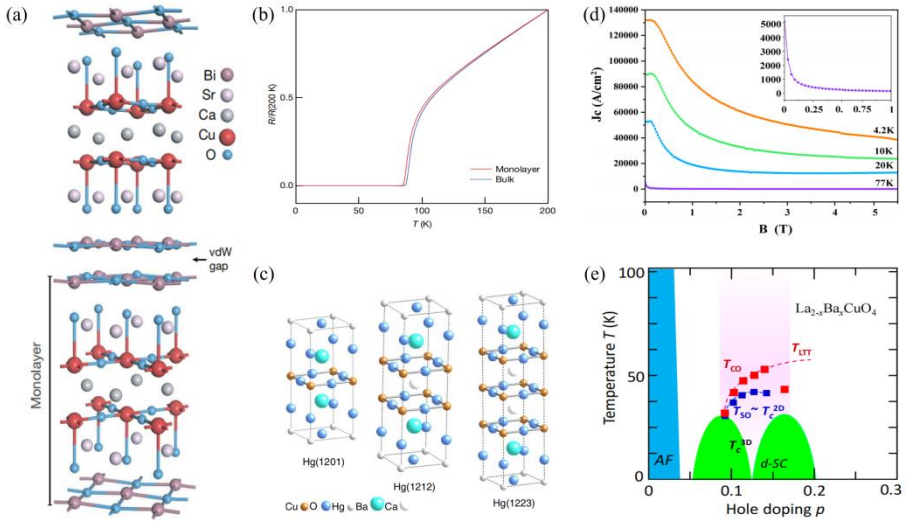

Figure 1. (a) Schematic diagram of the atomic structure of Bi-2212; (b) Typical temperature-dependent resistance of a single-layer Bi-2212 sample; (c) Crystal structures of three Hg-cuprate superconductors; (d) Field-dependence curves of critical current density at different temperatures; (e) Phase diagram of $La_{2-x}Ba_xCuO_4$ [4]

Wang et al. utilized a solid-state reaction method under a flowing oxygen atmosphere to synthesize the YbBa2Cu3O7−y (YBCO) superconductor, achieving a superconducting transition temperature of about 89.9 K [2]. The critical current density (J_c) in a self-field, calculated from the M-H curve, was over 130 kA/cm² at 4.2 K and dropped to about 5 kA/cm² at 77 K, as shown in Figure 1(d). Zhang et al. used the TSMG method to prepare YBCO samples with varying Ag2O doping levels and found that an appropriate amount of Ag2O doping could enhance the flux pinning landscape (FL) and reduce the relaxation rate, indicating that Ag doping effectively improves the superconducting properties of YBCO [3]. Bednorz and Müller utilized chemical doping techniques to prepare the La-Ba-Cu-O system. Subsequently, Tranquada et al. introduced stripe order into $La_{2-x}Ba_xCuO_4$ (LBCO) by Nd substitution and Ba doping. LBCO possesses a distinctive long-range, ordered three-dimensional spin-charge stripe order characteristic of the La214 family, which is clearly presented in the phase diagram shown in Figure 1(e) [4]. LBCO exhibits stripe order coexisting with superconductivity at low temperatures, and the strength of this order changes significantly with varying doping levels. The formation of stripe order is thought to be closely related to strong electronic correlations and lattice distortions [5], promoting an orderly arrangement of charge and spin. There is a competitive relationship between charge order and the superconducting state, thus, the manipulation of charge order through magnetic fields and pressure can directly affect the behavior of the superconducting state.

In summary, superconducting performance can be enhanced by improving crystal growth conditions, optimizing the copper-oxygen layer structure, and adjusting interlayer coupling to strengthen superconducting currents. Precise element doping, such as adjusting charge and spin order through external pressure or chemical doping, can increase the superconducting transition temperature and coherence. Improving growth techniques like Molecular Beam Epitaxy (MBE) can enhance the phase purity and uniformity of samples, thus enhancing superconducting stability. Moreover, combining theoretical calculations with experimental research is expected to uncover the mechanism of cuprate superconductivity and promote the practical application and development of high-temperature superconductivity technology.

3. Iron-based High-tempreature Superconductors

Iron-based high-temperature superconductors (FeSCs) are more appealing than traditional cuprate superconductors. The high critical temperatures of FeSCs and their ability to maintain superconductivity under strong magnetic fields offer broad prospects for applications in high-performance magnets and other fields. However, the electron pairing mechanism in FeSCs is complex and not fully understood, with significant differences likely between materials. Additionally, the lattice instability of FeSCs under high pressure may affect their superconducting properties, necessitating further research to enhance the stability of these materials.

Kamihara et al. synthesized a new type of iron-based superconducting material, LaOFeAs, through chemical doping. LaOFeAs features an alternating Pnictide layer structure of FeAs layers and charge-reshuffled layers, interconnected by different cations. Fa Wang et al. explored the superconducting properties and electron-pairing mechanisms of these materials through theoretical analysis and computational simulation. They found that with appropriate doping or pressure treatment, these materials could achieve a superconducting transition temperature as high as 55 K. The principle of their superconductivity may be related to electron pairing in the FeAs layer, with various possible pairing symmetries such as s-wave and d-wave. Figure 2(a) illustrates the crystal structure of iron-based superconductors, where Fe ions form a two-dimensional square lattice, and the Pnictide or Chalcogen layers are stacked alternately. Adroja et al. used the μSR technique to study $ACa_2Fe_4As_4F_2$ (A=K, Rb, Cs), which have a double-layer Fe_2As_2 structure and exhibit multi-band superconductivity. A two-gap model with line nodes shows strong coupling characteristics. The inverse square of the in-plane penetration depth as a function of temperature, as shown in Figure 2(b), does not conform to the form of an s-wave superconductor, but is well described by a two-band model with line nodes. Additionally, the zero-field μSR results shown in Figure 2(c) indicate that the material maintains time-reversal symmetry (TRS) in the superconducting state [6].

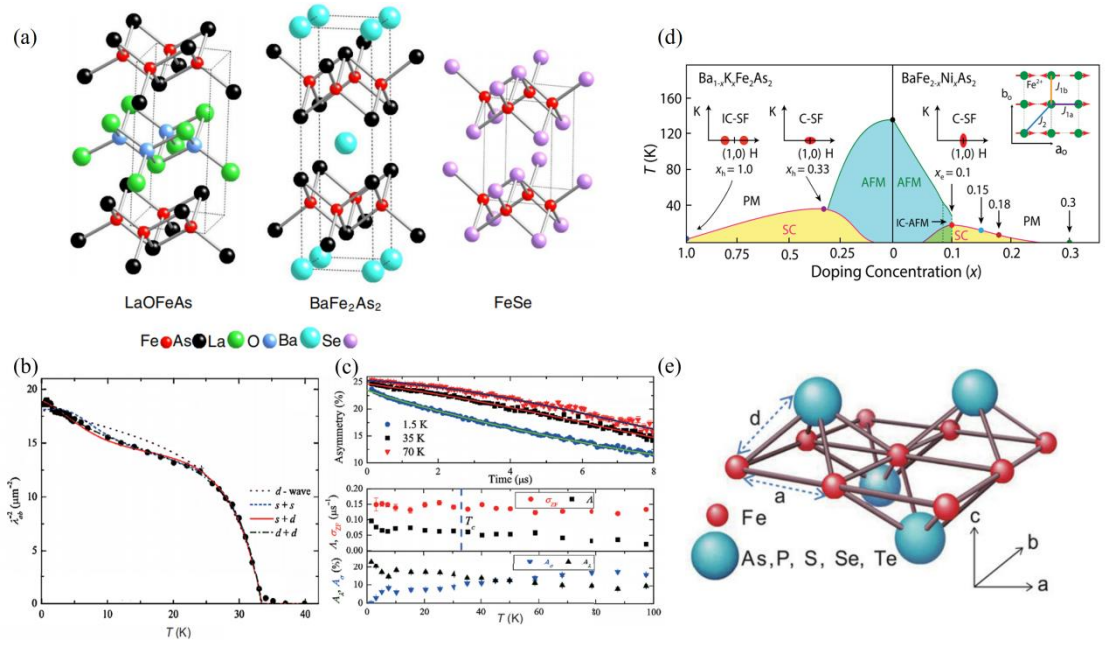

Figure 2. (a) Crystal structures of three iron-based superconductors; (b) The square of the penetration depth in the $KCa_2Fe_4As_4F_2$ plane as a function of temperature; (c) Time dependence of the zero-field muon spin relaxation spectrum of $KCa_2Fe_4As_4F_2$ at different temperatures; (d) Electronic phase diagram of electron-doped and hole-doped $BaFe_2As_2$; (e) Structure of the X-Fe-X trilayer [8]

Chen et al. achieved a superconducting transition temperature of 22K in $BaFe_2As_2$ through high-pressure treatment. Dai et al. used neutron scattering techniques to study the spin dynamics and antiferromagnetic order of these materials, suggesting that magnetism may be a common feature of the superconductivity in such materials [7]. Moreover, the superconducting transition temperature

can be tuned through doping, and as shown in Figure 2(d), the phenomenon of electron or hole doping significantly affecting the spin excitation spectrum of iron-based superconductors provides the possibility of optimizing superconducting properties through electronic structure control. Hao and Hu, through theoretical model analysis, studied the heterostrucure of single-layer FeSe/$SrTiO_3$ [8]. Figure 2(e) presents the X-Fe-X trilayer structure where the FeSe layer alternates with the substrate. When the interaction between FeSe and the substrate reaches a critical value, the material undergoes a topological phase transition, forming electronic states with nontrivial topological properties, which in turn affect the material's electronic structure. It may also enhance superconductivity by affecting the electron-phonon interaction. This phase transition and the formation of electronic states are closely related to the internal electronic structure and the topology of the Fermi surface.

Therefore, by doping rare or transition metal elements and regulate the Fermi surface topology, iron-based superconductors demonstrate their unique advantages and potential as high-temperature superconducting materials. Improving the crystal structure, such as substituting the Ca layer with Ca_2F_2 to adjust the nodal properties, provides an effective way to overcome the challenges of asymmetric pairing and time-reversal symmetry breaking, which helps to further enhance superconducting performance. Appropriate pressure control, combined with a deeper understanding of the interaction between spin excitations and superconductivity, can aid in designing superior new superconducting materials and promote their development towards practical applications.

4. Nickel-based Superconductors

Nickel-based high-temperature are similar to copper-based and iron-based superconductors. However, the harsh conditions for the material preparation of nickel-based superconductors and the difficulty of sample preparation have largely limited the development of nickel-based superconductors.

He et al. designed a Mo_2NiB_2 (Crystal structure as shown in Figure 3(a)) superconductor and analyzed the crystal structure of Mo_2NiB_2 by synchrotron radiation. Mo_2NiB_2 exhibits a superconductivity of 4K, and the non-stoichiometric ratio of Ni sites can control its T_c. The lack of Ni is favorable for superconductivity, but excessive Ni is detrimental to superconductivity and bias produces a suppression of superconductivity. The main carriers of Mo_2NiB_2 are electrons, and the vacancies of Ni are equivalent to hole doping decreasing the electron carrier concentration. Less hole doping helps superconductivity, and as the number of Ni vacancies increases further, the concentration of electron carriers decreases, and superconductivity is gradually restrained [9]. Hirofumi Sakakibara et al. theoretically investigated the superconducting properties of $La_3Ni_2O_7$ and it can reach a high T_c in the two-layer Hubbard model. The superconducting properties of $La_3Ni_2O_7$ can achieve high T_c in the two-layer Hubbard model, and have been calculated by the first principles and the linearized Eliashberg equation. The energy band structure of $La_3Ni_2O_7$ concluded that the system can be viewed as a double-layer Hubbard model for the d_{3z}^2-r^2 orbitals, and it can be formed between the orbitals reducing the superconductivity. The d_{3z}^2-r^2 portion of the electronic structure seems to favor superconductivity. it deviates from the ideal model, and can also be made to be superconducting by electron doping or by increasing ΔE and $|t_\perp|$ to make the electronic d_x^2-y^2 to d_{3z}^2-r^2 orbitals self-adulterated to improve the superconducting properties, as shown in Figure 3(b) [10]. Qu et al. studied the bilayer t-J-$J_\perp$ model of $La_3Ni_2O_7$ using a tensor network approach to find robust s-wave superconducting (SC) ordering mediated by interlayer magnetic coupling with a large pore density as well as a double-layer t-J-$J_\perp$ (The bilayer t-J-$J_\perp$ model is shown in Figure 3(c)) model with high T_c and strong antiferromagnetism (AF) interlayer exchange of $J_\perp$ may allow the presence of two eg orbitals in $La_3Ni_2O_7$: d_x^2-y^2 and d_z^2. The coupling of the FM Hund “bonds” the spins of the two eg orbitals to the d_x^2-y^2 electrons with strong spin transport. y^2 electrons conveying a strong AF coupling [11]. Huang et al. determined the superconducting order parameter by self-consistently solving the real-space Bogoliubov-de Gennes (BdG) equation, revealing robust and stable extended s-wave pairing symmetry [12]. It investigated the single impurity effect by using both the self-consistent BdG equation and a non-self-consistent T-matrix approach, showing the following the peak-to-peak structure of the local density of states at the vortex center and also explaining the low-energy gap

state. The numerical results show that impurity effects and vortex states can effectively be used to study the pairing symmetry of superconducting $La_3Ni_2O_7$ materials.

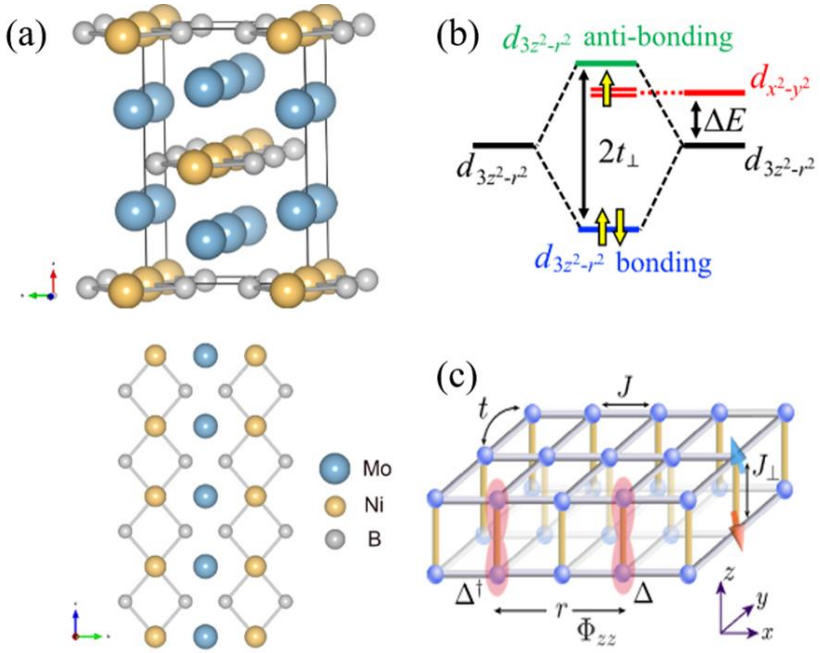

Figure 3. (a) Crystal structure of Mo_2NiB_2; (b) Energy diagram of the eg orbitals in the bilayer model; (c) The bilayer t-J-$J_\perp$ model [11]

In summary, tensor networks and other approaches to studying the double-layer model of nickel-based superconductors allow for the detection of their impurity effects and vortex states at the same time. The partial deletion of nickel produces less hole doping and it contributes to the further improvement of T_c. In addition, the self-hybridization of electrons from the $d_{x^2-y^2}$ to $d_{3z^2-r^2}$ orbitals can improve the superconducting properties, but the interorbital coupling in the bilayer Hubbard model decreases the superconductivity. The above methods can help to increase the T_c at the same time. It can be studied more deeply in nickel-based superconductors using theoretical calculations and simulations, and it is difficult to prepare the material.

5. Hydrogen-based Superconductors

Hydrogen-based superconductors have impressive high T_c. The T_c of some materials is close to room temperature under high-pressure conditions, much higher than that of other superconductors. However, the pressure required for hydrogen-based superconductors is much higher than the ambient pressure, making it difficult for them to become practical materials. It is still a great challenge to reduce the pressure required for hydrogen-based superconductors dramatically and effectively, it has not yet been overcome.

Zhang et al. designed a low-pressure, high-temperature body of ternary hydrogen-based superconductors with an alloyed main chain, and it is based on the principle of alloying with small-radius elements and hydrogen to form an alloy that replaces the H-H bonding [13]. The results show that the fluorite-type main-chain hydride structure has the potential to be room-temperature superconducting and that its dynamic stability is dependent on the radius of the pre-pressurized proto. The fluorite-type main chain is formed differently. In the unique bonding environment of the fluorite-type main chain in the unique bonding environment of fluorite-type host chains, a large amount of charge can be transferred to the H atoms as shown in Figure 4(c). These extra electrons can elongate the H-H bond and also lead to an increase in the density of H-derived states at the Fermi energy level. Kapildeb Dolui et al. studied a substable ambient-pressure hydride Mg_2IrH_6 superconductor, and it can be obtained by removing the interstitial H atoms from Mg_2IrH_7 [14]. A synthetic route utilizing high pressure may yield a substable ambient pressure phase. It remains substable upon return to lower

pressure due to its dynamic and kinetic stability. He et al. proposed to achieve high-temperature superconductivity at ambient pressures by injecting hydrogen into Pb to produce the stabilized hydrogen-poor dibasic chalcogenide Pb_4H (structure as Figure 4(d)), and they employ a first-principles approach and the Migdal-Eliashberg theory to study the structural stability, electronic properties, phonon spectrum, EPC and superconductivity of Pb_4H [15]. The vibration of hydrogen atoms induces several high-frequency optical phonon modes with relatively large phonon linewidths. Therefore, the strong anisotropy of the EPC strength can increase the critical temperature. The metallic bonding of Pb_4H ensures its excellent ductility compared to the UHP. In addition, the metal bond in Pb_4H ensures its excellent ductility, it is easier to produce than the ultrahigh-pressure polyhydrogen high-temperature superconductors because of its simple structure. Sun et al. investigated the structure and superconducting properties of rare-earth polyhydrogen compounds [16]. It is formed by the entire lanthanide system under pressure. They analyzed the electronic, kinetic, and electron-phonon coupling interactions in the hydroxide-rich hydrides. They have strong EPC interactions and high T_c superconductivity, and it is based on the principle of the atomic hydrogen cage structure of the hydrogen-rich packet with an atomic hydrogen structure. The high-frequency hydrogen sublattice vibrations of hydrogen-rich inclusion hydrides with atomic hydrogen cage structures effectively contribute to the strong EPC, and it enhanced superconductivity. A systematic study of electron-phonon coupling and superconducting T_c in all rare earth hydrides is lacking. They suggest that exploring the second island of late lanthanide polyhydrides may lead to the realization of room-temperature T_c.

He et al. make a new less hydrogen metal-bonded layered magnesium hydride $(Mg_4)_2H_1$ (structure as Figure 4(e)). It has strong electron-phonon coupling. It is fully metal-bonded at atmospheric pressure and exhibits excellent ductility and high-temperature superconductivity.The superconductivity of $(Mg_4)_2H_1$ arises from a novel high-frequency optical phonon branch [17]. It originates from the vibrations of the hydrogen atom and a relatively large phonon linewidth. Minko et al. implemented an unconventional protocol to probe the captured magnetic flux in H_3S and LaH_{10} at high pressures with magnetic measurements of superconductors in the superconducting quantum interferometry device SQUID magnetometer [18]. H_3S and LaH_{10} at high pressures do not have a significant Meissner effect. The advantage of this method is the magnetic response of the captured flux is virtually unaffected by background interferences from the DAC, and it includes background signals from the diamond anvil chamber and it is due to the absence of an external magnetic field. It enables effective differentiation of different phases in multiphase samples, detection of the critical current density, j_c and determination of Hc1. Sun et al. have investigated the magnetic response of ternary Na-P-H hydrides. They found two hydride superconductors, $NaPH_6$ and $NaPH_8$, examined their structures, and calculated the EPC and superconducting critical temperatures and T_c [19]. The results indicate that the high T_c of $NaPH_6$ at high pressure is due to the high density of H s states in the Fermi energy level, and the H atoms contribute to the strong EPC interactions in the ternary phosphorus hydrides. In addition, alkali and alkaline-earth metals can provide electrons. They can enhance the T_c of hydrides. Gao et al. discovered a strongly coupled superconductor, $CsBH_5$, based on density-functional theory (DFT) calculations. The modulation of virtual high-pressure is 1 Gpa, and it can be affected by the substitution-modulated charge transferring from metal atoms to hydrogen atoms. It enhances the structural stability and prohibits the reappearance of the $[BH_5]^{2-}$ anion. This mechanism can reduce the pressure without altering the crystal structure of hydrogen-rich compounds. Boron and hydrogen bonding is strong and boron is slightly less electronegative than hydrogen, and doping of boron hydride crystals with holes may lead to room-temperature superconductivity [20].

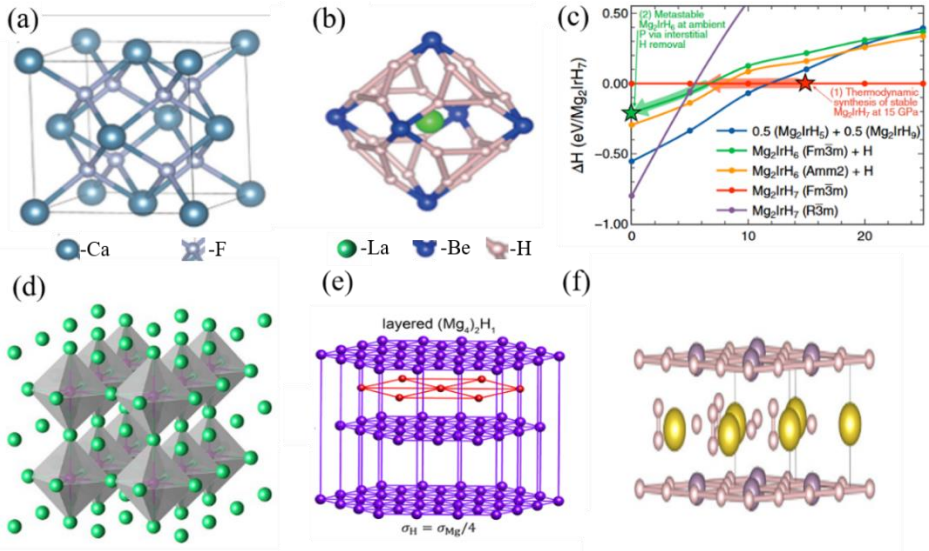

Figure 4. (a) Crystal structure of fluorite CaF_2; (b) Fluorite-type cage of $LaBeH_8$; (c) Pressure dependence of the enthalpy of formation of Mg-Ir-H; (d) Crystal structure of binary metal-bonded chalcogenide Pb_4H. (e) Schematic representation of $(Mg_4)_2H_1$ oligo-hydrogen metal-bonded layered magnesium hydride; (f) Supercells of $P\bar{6}m2$ $NaPH_6$ [17]

In summary, hydrogen-based superconductors have a higher T_c, but the high-pressure conditions can lead to severe limitations in superconductor applications. Chemical pre-compression can be used to generate valence densities of metallization at low pressures and synthesize ternary hydrogen-based superconductors. Alkali or alkaline-earth metals can be used to provide electron-enhanced T_c to form hydrogen-poor superconductors, and they can generate a strong EPC (electron-phonon coupling) to reduce the required pressures. In the case of hydrogen-rich superconductors, substitution can be used to regulate the charge transfer from the metal atoms to the hydrogen atoms to form virtual hydrogen-rich superconductors. It can retain the hydrogen-rich structure, drastically reduce pressures, and improve the application. For hydrogen-rich superconductors, the pressure drastically while retaining the hydrogen-rich structure can be reduced to improve the superconductivity.

6. Conclusion

High-temperature superconductors have a wide range of applications in fields such as electric power transport, electronic devices and quantum computing due to their higher critical temperature, zero resistance and antimagnetic properties. Therefore, this paper reviews the properties and mechanisms of copper-oxide, iron-based, nickel-based and hydrogen-based high-temperature superconductors. It is found that optimising the copper-oxygen layer structure and regulating the interlayer coupling are effective ways to improve the performance of copper oxide high temperature superconductors and enhance the superconducting current of the materials. By doping rare elements, transition metal elements and regulating the Fermi surface topology to change the internal electronic structure of iron-based high-temperature superconductors, and the superconducting transition temperature and energy gap of the materials are enhanced. Double-layer structure can be investigated by using tensor networks and other methods, to increase the T_c and solve the problems, such as the difficulty of material preparation for nickel-based high-temperature superconductors. Hydrogen-based high-temperature superconductors can be synthesised into ternary hydrogen-based superconductors and hydrogen-poor superconductors by using chemical pre-pressurisation and doping with alkali metal elements, and it can increases the transition temperature of the superconducting materials and reduces the pressure required for their preparation. Therefore, the present study is dedicated to the enhancement of the superconducting properties of copper oxide, iron-based, nickel-based, and hydrogen-based high-temperature superconductors to broaden their applications in a variety of fields,

such as electric power transport in production and life, electronic devices, and quantum computation in scientific research.

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