Research Progress of Hydrogen-rich Superconducting Materials under High Pressure

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Abstract. In recent years, hydrogen-rich high-temperature superconducting materials such as H3S and LaH10 discovered by scientists under ultra-high pressure have continuously broken the record of superconducting critical temperature, bringing hope for the ultimate realization of room-temperature superconductivity and thus attracting widespread attention. This article takes the timeline of the discovery of hydrogen-rich superconducting materials as the axis, summarizes the main superconducting material systems and microscopic mechanisms discovered so far, and focuses on introducing the current research progress, problems and challenges faced by high-temperature superconducting materials of hydrogen-rich compounds, providing possible research ideas for the future.

Keywords: hydride superconductors, high-pressure synthesis, room-temperature superconductivity, electron-phonon coupling, chemical pre-compression.

1. Introduction

Since scientistss discovered in 1911 that mercury exhibits zero resistance at 4.2 K [1], superconductivity research has been a central focus in condensed matter physics. The zero resistance and perfect diamagnetism (Meissner effect) of superconductors confer significant potential for applications in energy transmission, magnetic levitation, and quantum computing [2]. However, the critical temperature (Tc) of conventional superconductors is extremely low, typically requiring cooling with liquid helium (4.2 K) or liquid nitrogen (77 K), which limits their practical applications. Therefore, achieving room-temperature superconductivity ($Tc \geq 300$ K) has become the ultimate goal of the scientific community.

Hydrogen-rich superconducting materials refer to compounds formed by combining hydrogen with other elements under high-pressure conditions, exhibiting superconductivity; their superconducting mechanisms, material design, and potential applications are focal points in current superconductivity research. This article systematically introduces the discovery and development of hydrogen-rich superconducting materials, elucidates the mechanisms of their metallization and high-temperature superconductivity, and highlights the current difficulties and challenges.

2. Discovery and Development of Hydrogen-Rich Superconducting Materials

Hydrogen does not exhibit superconductivity at ambient temperature and pressure; however, under high pressure, hydrogen forms hydrides which can exhibit superconductivity under specific conditions. In 1968, Ashcroft first theoretically discussed the possibility of achieving high-temperature superconductivity in solid metallic hydrogen [3]; Following the development of BCS theory, Ashcroft further proposed the concept of 'chemical precompression' in 2004, suggesting that metallic hydrogen and its compounds could serve as ideal high-temperature superconducting materials [4]. However, to date, due to the extremely stringent requirements of metallic hydrogen on high-pressure experimental techniques, its superconducting properties have not been experimentally confirmed. In the 1980s, scientists proposed that hydrides might exhibit superconductivity, but it was not until recent breakthroughs in high-pressure experimental techniques that hydrogen-rich superconductivity was truly observed.

One of the most notable features of hydrogen-rich superconducting materials is the significant enhancement of their superconducting transition temperature. In 2015, Drozdov and Eremets' team at the Max Planck Institute for Chemistry, Germany, successfully synthesized a hydrogen-rich superconducting material—H3S (sulfur hydride)—and observed a superconducting transition temperature of 203 K (–70 °C) under an extremely high pressure of 150 GPa, a temperature far exceeding that of conventional superconducting materials [5]. In 2017, studies showed that the superconducting transition temperature of the cage-like hydride LaH10 under high-pressure conditions exceeded 250K, approaching the ideal goal of room-temperature superconductivity.

From 2011 to 2014, several theoretical research groups, both domestic and international, predicted that the superconducting temperature of the novel hydrogen-rich hydride H3S could surpass 200 K ; Subsequently, the Eremets group at the Max Planck Institute for Chemistry, Germany, synthesized hydrogen sulfide (H3S) at 150 GPa and observed superconducting properties at 203 K, exceeding the liquid nitrogen temperature region and consistent with theoretical predictions [6]. This discovery not only demonstrates that the strong electron-phonon coupling mechanism remains applicable in hydrogen-rich systems, but also sparked a surge of research interest in hydrogen-rich compounds. The success of H3S indicates that, through chemical precompression (i.e., introducing other elements to form compounds with hydrogen), the pressure required for hydrogen metallization can be significantly reduced, thereby providing a new pathway for exploring high-temperature superconductivity.

In 2017, Ma Yanming and Liu Hanyu each predicted based on first principles that the Tc of cage-like LaH_{10} could reach 280 K at the 170 GPa level, just one step away from the critical point at room temperature. [7]In 2019, the Eremets group measured samples of the same structure with a diamond anvil cell and confirmed that Tc = 250 K, once again setting a new record for hydrogen-rich superconductivity and approaching room-temperature superconductivity. The high critical temperature of this system is attributed to the efficient charge injection of La into the H_{32} framework, which hardens the high-frequency phonons of the hydrogen sublattice and strongly couples them with the Fermi surface electrons, causing a sudden increase in the λ value. According to the Allen-Dynes formula, Tc thus rises significantly.[8].

These breakthroughs indicate that hydrogen-rich materials, through chemical preloading, can not only reduce the pressure required for hydrogen metallization but also achieve a higher superconducting transition temperature by optimizing the electron-phonon coupling strength. In addition, the diversity of hydrogen-rich compounds (such as binary, ternary and polyhydrides) provides a broad space for material design. For instance, by introducing light elements (such as lithium and magnesium) or transition metals (such as lanthanum and cerium), the electronic structure and lattice dynamics of the material can be further regulated, thereby optimizing superconducting performance.

3. Microscopic Mechanism of Hydrogen-Rich High-Temperature Superconductivity

With the continuous research on hydrogen-rich superconductivity developing, hydrogen-containing compounds have successively broken the records of superconducting transition temperatures and are constantly approaching room temperature under the condition of millions of atmospheres,.

Hydrogen-rich superconductors have theoretical mechanisms within the framework of BCS superconductivity theory as every others typical traditional superconductors, Electrons form pairs through interactions with lattice vibrations (phonons), thereby generating superconductivity. Under high pressure conditions, hydrogen atoms in hydrides may lead to stronger electron-phonon interactions, thereby increasing the superconducting temperature.

The properties of hydrogen atoms play a significant role in the phenomenon of hydrogen-rich superconductivity: under high pressure conditions, the electron cloud of hydrogen changes, promoting the development of superconductivity by forming new chemical bonds or modifying the lattice structure. Hydrogen atoms in hydrides may generate superconductivity by creating local fluctuations in electron density. Recent studies also indicate that quantum effects such as the zero-point vibration of hydrogen may have a significant impact on stability and superconducting performance. Therefore, it can be considered that hydrogen atoms are the core factor driving hydrogen-rich systems to reach superconducting conditions close to room temperature [9]. Therefore, in hydrogen-rich superconducting materials, hydrogen atoms provide high-frequency phonons to the system, which in turn can enhance the electron-phonon coupling and increase the transition temperature of superconductivity.

In the realization of hydrogen-rich superconductivity, high-pressure conditions are indispensable. Under high pressure conditions, it can significantly shorten the bond lengths between hydrogen atoms, enhance the overlap of electron orbitals, and thereby promote the metal-like properties of hydrogen. The interaction between hydrogen atoms will change, which may lead to the reconstruction of electronic states and enhance the ability of superconducting pairing. Therefore, superconductivity not only depends on the chemical composition of the material, but is also affected by the applied pressure. We can also consider that the high-pressure effect is a necessary condition for achieving high Tc superconductivity in hydrogen-rich materials.

4. Research Challenges of Hydrogen-Rich Superconducting Materials

4.1 Stability under high-pressure conditions

Hydrogen-rich superconducting materials typically require extremely high-pressure conditions to exhibit superconductivity. For instance, in hydrides (such as H3S), superconductivity is generally realized only under high pressures of several hundred gigapascals (GPa). These high-pressure conditions far exceed the capabilities of conventional laboratory equipment, and most hydrogen-rich superconducting materials are unstable at ambient temperature and pressure. Therefore, a major current research challenge is how to synthesize stable hydrogen-rich superconducting materials at lower pressures or how to preserve their superconductivity under ambient pressure.

4.2 Realization of High-Temperature Superconductivity

Currently, the superconducting transition temperatures of hydrogen-rich superconducting materials have achieved significant breakthroughs (for example, LaH10 exhibits a superconducting transition temperature of 250 K under high pressure), but they remain far from achieving room-temperature superconductivity. Realizing room-temperature superconductivity, especially at ambient pressure, is an immense challenge.

4.3 Synthesis and Preparation Challenges

The synthesis of hydrogen-rich superconducting materials generally requires extremely stringent experimental conditions. In particular, during the synthesis of hydrides or hydrogen-rich compounds under high pressure, specialized high-pressure apparatuses such as diamond anvil cells (DACs) are used. Even under the conditions mentioned above, the synthesis process of the material remains extremely complex and precise, with a low yield, and can only synthesize samples at the micrometer level. The low preparation amount of the material limits the possibility of in-depth research on its performance. Especially even if it is successfully synthesized under high pressure, some materials will still rapidly decompose or transform into non-superconducting phases during the depressurization process, making it difficult to maintain stability[4]

4.4 Behavior and Chemical Stability of Hydrogen

Hydrogen, as the lightest chemical element, has very complex and diverse behaviors in different chemical environments. Under high pressure conditions, hydrogen atoms often exhibit complex arrangements and even show competition between molecular states and atomic states[10]. The degree of charge transfer and the chemical potential of hydrogen in different chemical environments have significant impacts on the stability of the crystal structure, the density of states of electrons, and the electron-phonon coupling. Under high pressure conditions, hydrogen atoms may also undergo bond topology rearrangemen, affecting the structural stability of hydrogen-rich superconducting materials. Therefore, the crystal structure of hydrides under high pressure is extremely complex. How to understand the role of hydrogen in superconducting materials and how to control the structure and composition of the materials are the difficulties in further research. It can be seen from this that if further breakthroughs are to be made in the research of hydrogen-rich superconductivity, the core issue is to deeply understand the microscopic role of hydrogen in hydrogen-rich superconducting materials and formulate effective strategies to "improve their kinetic stability or reduce the required synthesis pressure.

4.5 High-Pressure Synthesis and Characterization

At present, the research on hydrogen-rich superconductivity is still restricted by the strict constraints of high-pressure environments. The experimental equipment for hydrogen-rich superconducting materials is extremely expensive and the operation is complex. Firstly, typical systems such as H3S and LaH10 can only achieve stable superconductivity in the range of 150 to 200 GPa. Extreme high-pressure conditions (usually exceeding 100 GPa) impose extremely high demands on experimental equipment and techniques. Moreover, after depressurization, the materials rapidly decompose or lose hydrogen, and the metastable retention strategy at normal temperature and pressure is still not mature. Secondly, there are many difficulties in the synthesis of materials under high pressure, such as the small volume of the sample chamber and low output. The chamber of the diamond anvil cell (DAC) is less than 10-4mm^3, the reaction window is narrow, and the precision requirement for temperature-pressure coupling control is extremely high. Moreover, the sample is prone to degradation during temperature recovery or pressure relief, resulting in poor repeatability and extremely low yield. Finally, there are also many difficulties in characterizing materials under high pressure. To obtain more accurate data, it is necessary to combine multiple technical means, such as X-ray diffraction, magnetic measurement, etc. The DAC needs to be integrated with low-temperature strong magnetism, synchrotron radiation or neutron beam lines. The equipment is expensive and the operation is complex, and the signal detection sensitivity is low. This makes the research process more difficult and consumes more resources. In conclusion, although the record Tc has broken through 260K and is only 13K away from room temperature, due to the significant distance from true room-temperature superconductivity, the technical bottlenecks of high-pressure synthesis and characterization still hinder the systematic research and subsequent large-scale production of hydrogen-rich superconductors.

5. Conclusion

Hydrogen-rich superconducting materials, as a frontier in superconducting research, have made significant progress both theoretically and experimentally. Although current research still faces issues such as high-pressure conditions, synthesis techniques and stability, its potential application prospects are highly anticipated. With the continuous development of science and technology, hydrogen-rich superconducting materials are expected to achieve high-temperature superconductivity at normal temperature and pressure in the future, promoting innovations in multiple fields such as energy and quantum computing.

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