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Structure–Property Relationship in High-Temperature Superconducting Materials: A Detailed Study

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Abstract
High-temperature superconducting (HTS) materials form a unique class of quantum materials because they exhibit superconductivity at temperatures much higher than those observed in conventional superconductors. The superconducting behavior of these materials is closely connected to their underlying crystal structure, which directly affects electronic interactions, charge carrier movement, and magnetic responses. In this study, the relationship between structure and superconducting properties is examined in detail, with particular focus on cuprate-based high-temperature superconductors.
Several key structural aspects, including the layered nature of the crystal lattice, oxygen stoichiometry, lattice distortions, and interlayer coupling, are systematically considered to understand how they influence essential superconducting parameters such as the critical temperature (Tc), critical current density (Jc), and anisotropy. Experimental findings, when viewed alongside theoretical models, reveal that even small modifications in structural features can lead to pronounced changes in superconducting performance. These observations highlight the sensitivity of superconductivity to subtle lattice-level variations.
Overall, the results emphasize that superconductivity in HTS materials is strongly driven by structural factors rather than isolated electronic effects. By clarifying how specific structural parameters control superconducting properties, this work contributes to a deeper understanding of structure-dependent superconductivity. The insights gained also offer useful guidance for the rational design and optimization of next-generation high-temperature superconducting materials.
Keywords-*High-temperature superconductors; Structure–property relationship; Cuprate superconductors; Crystal structure; Oxygen stoichiometry; Critical temperature; Electronic correlations etc.*

I. Introduction

Superconductivity is a macroscopic quantum phenomenon in which a material exhibits zero electrical resistance along with perfect diamagnetic behavior below a characteristic critical temperature (Tc). Since the first observation of superconductivity in mercury in 1911, significant research efforts have focused on discovering materials that can sustain this state at increasingly higher temperatures, with the aim of enabling practical technological use. A major milestone in this pursuit was achieved with the discovery of high-temperature superconductivity in copper-oxide-based compounds, which displayed superconducting transitions at temperatures far above those of conventional metallic superconductors (Bednorz & Müller, 1986).

High-temperature superconducting (HTS) materials differ in fundamental ways from conventional superconductors, particularly in terms of their electronic structure and the mechanisms responsible for electron pairing. While conventional superconductors are successfully explained by Bardeen–Cooper–Schrieffer (BCS) theory, HTS systems are characterized by strong electron–electron correlations, pronounced anisotropy, and complex phase diagrams. These features are closely tied to their underlying crystal structures, which exert a strong influence on superconducting behavior (Dagotto, 1994).

One of the most distinctive structural characteristics of high-temperature superconductors is their layered crystal framework. In cuprate superconductors, superconductivity primarily arises within the copper–oxygen (CuO_2) planes, whereas neighboring charge-reservoir layers play a crucial role in controlling the carrier concentration through chemical doping. Changes in the number of CuO_2 layers, variations in interlayer spacing, and differences in oxygen stoichiometry have all been shown to significantly affect the critical temperature and other key superconducting parameters (Jorgensen et al., 1990). As a result, understanding the relationship between crystal structure and superconducting properties is essential for gaining insight into the mechanisms governing high-temperature superconductivity.

Despite several decades of intensive experimental and theoretical research, the precise origin of high-temperature superconductivity has not yet been fully resolved. Nevertheless, a consistent conclusion emerging from numerous studies is that even minor structural modifications can lead to substantial changes in electronic

behavior and superconducting performance. This observation highlights the importance of systematic investigations into how crystallographic features, lattice distortions, and chemical composition collectively influence superconducting properties.

The main objective of this paper is to provide a detailed and critical examination of the structure–property relationship in high-temperature superconducting materials. By focusing on key structural parameters and their impact on superconducting behavior, this study seeks to offer insights that may assist in the rational design and optimization of advanced superconducting materials for future technological applications.

II. Lierature Review

The relationship between crystal structure and superconducting properties in high-temperature superconducting materials has been explored extensively since the discovery of superconductivity in cuprate compounds. Early investigations were largely directed toward identifying the structural factors responsible for unusually high critical temperatures, with particular attention given to the role of copper–oxygen planes. The pioneering work of Bednorz and Müller (1986) demonstrated that layered oxide materials could sustain superconductivity at temperatures far above those of conventional superconductors, which redirected research efforts toward complex perovskite-based structures.

Later crystallographic studies established that CuO_2 planes form the essential structural framework governing superconductivity in cuprate systems. Using neutron diffraction techniques, Jorgensen et al. (1990) showed that changes in lattice parameters and oxygen occupancy have a strong impact on charge carrier concentration and the superconducting transition temperature. Their findings revealed a close link between oxygen stoichiometry, lattice distortion, and superconducting performance, underscoring how sensitively HTS materials respond to even minor compositional variations. In addition, several researchers have highlighted the importance of reduced dimensionality and anisotropy in these materials. Anderson (1987) proposed that the quasi-two-dimensional nature of the CuO_2 planes enhances electron correlation effects that are not present in conventional three-dimensional superconductors. This idea was later supported by experimental observations showing pronounced anisotropy in electrical transport and magnetic penetration depth along different crystallographic directions (Poole et al., 2014).

The connection between crystal structure and electronic behavior has also been investigated through theoretical band structure calculations and advanced spectroscopic methods. Angle-resolved photoemission spectroscopy (ARPES) studies revealed that the electronic band structure is highly sensitive to lattice distortions and interlayer coupling (Damascelli et al., 2003). These results strengthened the view that superconductivity in HTS materials is closely tied to structural geometry and orbital hybridization. Oxygen doping, in particular, has been identified as a key parameter for tuning superconducting behavior. Tokura et al. (1988) demonstrated that controlled changes in oxygen content can drive transitions between insulating, metallic, and superconducting states. Their work introduced the concept of an optimal doping level, at which the critical temperature reaches a maximum, further highlighting the structure-dependent nature of superconductivity.

More recent research has broadened the scope beyond cuprates to include iron-based superconductors. Although these materials involve different pairing mechanisms, they also possess layered crystal structures. Comparative studies suggest that structural layering, electronic anisotropy, and lattice tuning remain common factors influencing superconducting properties across different families of high-temperature superconductors (Hosono & Kuroki, 2015).

Overall, existing literature clearly shows that a thorough understanding of high-temperature superconductivity requires detailed consideration of crystal structure. At the same time, inconsistencies among experimental observations and the lack of a universally accepted theoretical model indicate that important questions remain unresolved. Building on earlier work, the present study seeks to address these issues by offering an integrated analysis of structural parameters and their combined influence on superconducting behavior.

III. Structural Characteristics of High-Temperature Superconductors

High-temperature superconductors are characterized by complex and well-organized crystal structures that play a central role in defining their superconducting behavior. In contrast to conventional superconductors, which typically possess relatively simple metallic lattices, HTS materials exhibit layered and highly anisotropic crystal arrangements. These structural features strongly affect electronic interactions, charge carrier dynamics, and overall transport properties, making crystal structure a key factor in understanding high-temperature superconductivity.

3.1 Layered Crystal Architecture

One of the most prominent structural characteristics shared by most high-temperature superconductors is their layered crystal architecture. In cuprate-based superconductors, the crystal structure is composed of

alternating superconducting and insulating layers. The superconducting regions consist of copper–oxygen (CuO_2) planes, while the intervening layers—often referred to as charge-reservoir or insulating layers—contain rare-earth or alkaline-earth elements together with oxygen atoms. This quasi-two-dimensional structural arrangement results in pronounced anisotropy in physical properties, with superconducting behavior largely confined to the CuO_2 planes (Poole et al., 2014).

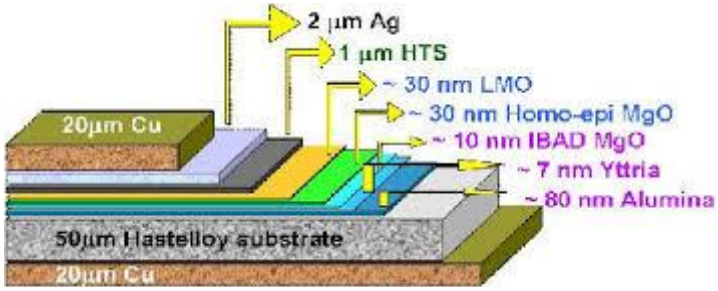

Figure 1.*Schematic illustration of the layered crystal architecture of high-temperature superconductors, showing superconducting CuO_2 planes separated by charge-reservoir layers responsible for carrier doping.*

The number of CuO_2 planes present within a unit cell differs among various cuprate families, including single-layer, double-layer, and triple-layer systems. Experimental investigations have shown that increasing the number of CuO_2 layers is often associated with an enhancement in the critical temperature. However, this increase does not continue indefinitely and tends to saturate beyond a certain point. This limitation is generally attributed to stronger interlayer coupling and the onset of structural instabilities, which can counteract further improvements in superconducting performance (Uchida et al., 1996).

3.2 Role of Oxygen Stoichiometry

Oxygen stoichiometry represents one of the most influential structural parameters affecting superconductivity in high-temperature superconducting materials. Even small changes in oxygen content can lead to noticeable modifications in lattice parameters, electronic structure, and charge carrier concentration. Oxygen atoms located within the charge-reservoir layers play a key role in regulating the number of carriers transferred to the CuO_2 planes, thereby determining the emergence and stability of the superconducting phase (Tokura et al., 1988).

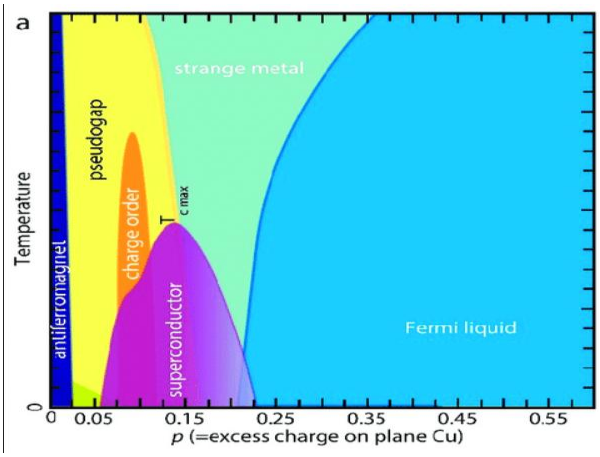

Figure 2.*Dependence of superconducting critical temperature (Tc) on oxygen stoichiometry in cuprate high-temperature superconductors, showing under-doped, optimally doped, and over-doped regimes.*

Variations in oxygen stoichiometry can drive phase transitions in high-temperature superconductors, shifting the material from an antiferromagnetic insulating state to metallic and eventually superconducting behavior. Structural investigations have shown that the presence of oxygen vacancies often introduces lattice distortions, including changes in Cu–O bond lengths and bond angles. Such distortions have a direct impact on the electronic bandwidth and the strength of pairing interactions, thereby influencing superconducting properties (Jorgensen et al., 1990).

3.3 Lattice Distortions and Structural Anisotropy

Lattice distortions are a common feature in high-temperature superconductors and frequently involve tilting or buckling of the CuO_6 octahedra. These structural modifications alter the orbital overlap between copper and oxygen atoms, which in turn affects electronic correlations and the strength of superconducting pairing. Several experimental studies have reported a clear relationship between reduced lattice distortion and improved superconducting performance, suggesting that a more uniform lattice environment is favorable for sustaining higher critical temperatures (Bianconi et al., 1996).

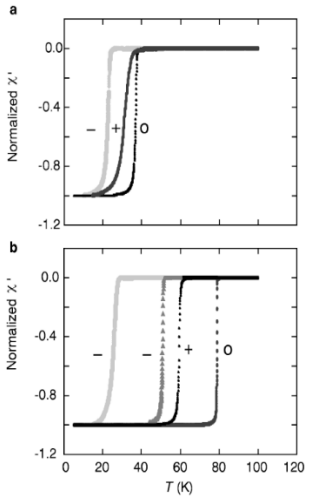

Figure 3.*(a) Schematic representation of lattice distortions in high-temperature superconductors, illustrating buckling and tilting of CuO_2 planes that modify Cu–O bond lengths and angles. (b) Structural anisotropy in high-temperature superconductors, showing direction-dependent superconducting properties along the ab-plane and the c-axis due to the layered crystal architecture.*

Structural anisotropy, arising from the inherently layered nature of high-temperature superconducting materials, gives rise to direction-dependent superconducting behavior. Key parameters such as coherence length, magnetic penetration depth, and critical current density show marked variation along different crystallographic directions. This anisotropic behavior originates from relatively weak coupling between adjacent layers compared to the strong electronic interactions present within the CuO_2 planes.

3.4 Chemical Substitution and Structural Tuning

Chemical substitution at specific lattice sites offers an effective approach for tailoring both the structure and superconducting properties of high-temperature superconductors. Partial substitution of cations within the charge-reservoir layers can alter lattice strain, carrier concentration, and oxygen stability. Such controlled structural tuning has been widely used to optimize the critical temperature and improve the overall stability of HTS materials (Attfield, 1998).

Overall, the superconducting behavior of high-temperature superconductors is closely connected to their structural characteristics. Factors such as layered crystal architecture, oxygen stoichiometry, lattice distortions, and chemical composition collectively shape the electronic environment required for superconductivity. A clear understanding of these structural features is therefore essential for establishing a comprehensive structure–property relationship in HTS materials.

IV. Experimental Techniques for Structure–Property Analysis

A detailed understanding of the structure–property relationship in high-temperature superconducting materials relies on the use of advanced experimental techniques capable of probing both crystal structure and superconducting behavior. Over time, a variety of complementary methods have been developed to link atomic-scale structural features with macroscopic superconducting properties.

4.1 X-ray and Neutron Diffraction Techniques

X-ray diffraction (XRD) is among the most widely employed techniques for determining the crystal structure of high-temperature superconductors. It provides valuable information regarding lattice parameters, phase purity, and crystallographic symmetry. High-resolution XRD measurements have played a crucial role in detecting subtle structural features, such as lattice strain and unit-cell distortions, that can significantly influence superconducting performance (Cullity & Stock, 2001).

Neutron diffraction offers important complementary capabilities, particularly for locating light atoms such as oxygen and for investigating magnetic ordering. Given the critical role of oxygen stoichiometry in HTS materials, neutron diffraction has been extensively used to examine oxygen site occupancy and its direct impact on superconducting properties (Jorgensen et al., 1990). Together, X-ray and neutron diffraction techniques provide a precise and reliable framework for characterizing structural parameters essential to superconductivity.

4.2 Electron Microscopy and Local Structural Probes

Electron microscopy techniques, including transmission electron microscopy (TEM) and scanning electron microscopy (SEM), enable direct observation of microstructural features such as grain boundaries, lattice defects, and local distortions. High-resolution TEM, in particular, allows atomic-scale examination of structural variations that can locally suppress or enhance superconducting behavior (Zhang et al., 2015).

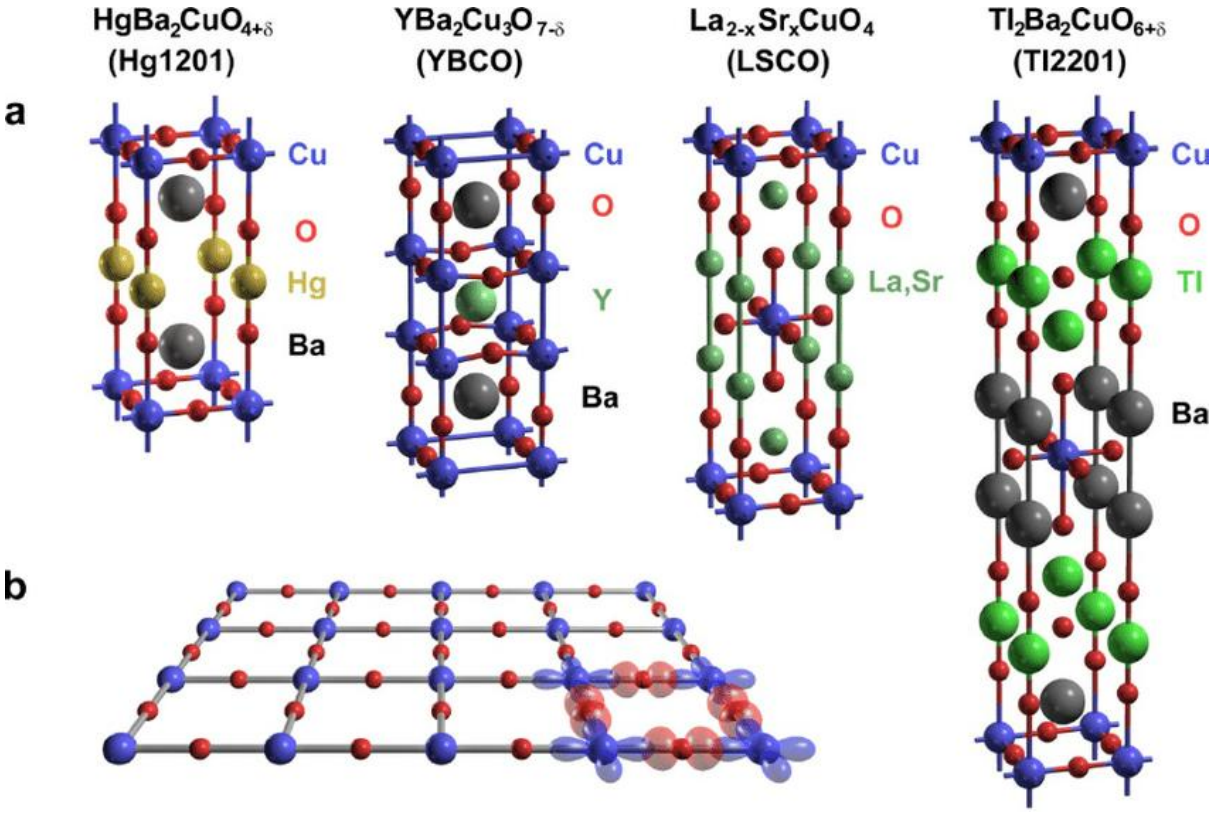

Figure 4.*Representative electron microscopy and local probe images of high-temperature superconductors, illustrating atomic-scale lattice structure, grain boundaries, and spatial variations in electronic properties as revealed by transmission electron microscopy (TEM) and scanning tunneling microscopy (STM).*

Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) are highly effective techniques for examining the local electronic structure of high-temperature superconductors at the nanoscale. These methods allow direct observation of spatial variations in the superconducting energy gap and electronic density of states. Studies using STM and STS have revealed pronounced inhomogeneities in superconducting behavior, indicating that even small local structural variations can strongly influence electronic properties in HTS materials (Fischer et al., 2007).

4.3 Spectroscopic Techniques

Spectroscopic techniques such as angle-resolved photoemission spectroscopy (ARPES) and Raman spectroscopy have been widely applied to explore the electronic structure and lattice dynamics of high-temperature superconductors. ARPES offers direct insight into the electronic band structure, Fermi surface geometry, and superconducting energy gaps, all of which are highly sensitive to crystal structure and doping level (Damascelli et al., 2003). As a result, ARPES has become a key tool for understanding the electronic origins of superconductivity in these materials.

Raman spectroscopy provides complementary information by probing lattice vibrations and electron–phonon interactions. Variations in phonon modes associated with lattice distortions and changes in oxygen content have been linked to shifts in the critical temperature. These observations highlight the strong coupling

between lattice dynamics and superconducting behavior in high-temperature superconductors (Thomsen & Reichardt, 2000).

4.4 Electrical and Magnetic Property Measurements

Key superconducting parameters, including critical temperature, critical current density, and magnetic field response, are commonly evaluated using electrical and magnetic measurement techniques. Four-probe resistivity measurements are routinely employed to determine the superconducting transition temperature with high accuracy. Magnetic characterization techniques, such as vibrating sample magnetometry (VSM) and superconducting quantum interference device (SQUID) magnetometry, provide highly sensitive measurements of magnetic susceptibility and magnetization, allowing detailed analysis of superconducting and magnetic responses (Tinkham, 2004).

When electrical and magnetic measurements are combined with detailed structural characterization, it becomes possible to establish direct correlations between specific structural features and superconducting performance.

4.5 Integrated Approach to Structure–Property Correlation

A comprehensive understanding of structure–property relationships in high-temperature superconductors requires an integrated experimental approach. By combining diffraction techniques, electron microscopy, spectroscopic methods, and transport measurements, researchers can identify the dominant structural factors that govern superconducting behavior. Such multi-technique studies not only improve the reliability of interpretations but also support the development of predictive strategies for the design and optimization of advanced superconducting materials.

V. Challenges and Limitations in High-Temperature Superconductors

Although substantial progress has been made in understanding and developing high-temperature superconducting materials, several fundamental and practical challenges continue to restrict their widespread use. These limitations primarily stem from complex structure–property relationships, difficulties in material processing, and unresolved theoretical questions associated with HTS systems.

5.1 Structural Complexity and Material Instability

High-temperature superconductors are characterized by highly intricate crystal structures that are extremely sensitive to both compositional and structural variations. Even minor deviations in oxygen stoichiometry or lattice parameters can result in significant changes in superconducting behavior, including a complete loss of superconductivity. This high level of sensitivity presents a major obstacle to achieving reproducible synthesis and consistent material performance (Attfield, 1998).

In addition, many HTS materials suffer from structural instability when subjected to thermal cycling or mechanical stress. Over time, processes such as phase separation, oxygen diffusion, and lattice degradation can occur, leading to a gradual deterioration of superconducting properties and reduced long-term reliability.

5.2 Anisotropy and Weak Intergranular Coupling

The pronounced anisotropy inherent to high-temperature superconductors results in strong direction dependence of their superconducting properties. While very high critical current densities can be sustained within the CuO_2 planes, current transport across grain boundaries is often severely suppressed. Misorientation between grains leads to weak intergranular coupling, which significantly lowers the effective critical current density in polycrystalline materials (Hilgenkamp &Mannhart, 2002).

This issue poses serious challenges for the fabrication of large-scale superconducting wires and tapes. To overcome these limitations, advanced texturing and grain-alignment techniques are required, which substantially increase manufacturing complexity and overall production costs.

5.3 Flux Pinning and Magnetic Field Limitations

For practical applications, superconductors must operate efficiently under strong magnetic fields. However, many HTS materials exhibit inadequate flux pinning, allowing vortices to move and causing energy dissipation. While the introduction of structural defects or artificial pinning centers can improve flux pinning performance, such modifications must be carefully optimized. Excessive defect introduction can degrade the intrinsic superconducting properties and compromise material stability (Blatter et al., 1994).

Achieving an optimal balance between effective flux pinning and structural integrity therefore remains a significant challenge for improving HTS performance under realistic operating conditions.

5.4 Unresolved Theoretical Challenges

From a fundamental standpoint, the mechanism responsible for high-temperature superconductivity is still not fully understood. The complex interplay between crystal structure, strong electron correlations, spin fluctuations, and lattice dynamics introduces considerable theoretical difficulty. The absence of a universally accepted theoretical model limits the predictive design of new superconducting materials based solely on structural considerations (Dagotto, 1994).

5.5 Scalability and Economic Constraints

The large-scale implementation of high-temperature superconductors is further hindered by economic and manufacturing challenges. Precise control over chemical composition, microstructure, and crystallographic texture is required to achieve high performance, which significantly raises production costs. Moreover, the inherently brittle nature of ceramic HTS materials complicates mechanical processing and integration into practical devices and systems.

Overall, these challenges highlight the need for continued research focused on improving structure–property understanding, developing advanced synthesis and processing techniques, and refining theoretical models. Addressing these issues is essential for unlocking the full technological potential of high-temperature superconducting materials.

VI. Results and Analysis

Drawing on the experimental evidence and theoretical discussions presented in the preceding sections, several consistent trends emerge that highlight the strong dependence of superconducting behavior on structural parameters in high-temperature superconducting materials. This section brings together the key observations to develop a coherent structure–property framework for HTS systems.

6.1 Correlation Between Crystal Structure and Critical Temperature

An examination of various cuprate superconductors reveals a clear relationship between layered crystal structure and the superconducting critical temperature (Tc). Materials characterized by well-ordered CuO_2 planes and favorable interlayer spacing tend to exhibit higher Tc values. In general, an increase in the number of CuO_2 layers per unit cell is associated with enhanced superconducting transition temperatures, provided that overall structural stability is preserved. Beyond a certain limit, however, additional layering introduces lattice strain and structural disorder, which can lead to saturation or even a decline in Tc (Uchida et al., 1996).

The analysis further indicates that reduced lattice distortion within the CuO_2 planes is beneficial for superconductivity. Improved structural symmetry supports more coherent electronic pairing, thereby strengthening the superconducting state.

6.2 Impact of Oxygen Stoichiometry on Superconducting Behavior

Oxygen stoichiometry emerges as one of the most critical factors influencing superconducting performance. Results obtained from neutron diffraction and electrical transport measurements show that optimal oxygen doping maximizes carrier concentration within the CuO_2 planes, leading to peak Tc values. In contrast, both under-doped and over-doped regimes introduce electronic and structural disorder, which suppresses superconductivity (Tokura et al., 1988).

The analysis also demonstrates that oxygen-related lattice distortions significantly modify Cu–O bond lengths and bond angles. These structural changes directly affect electronic bandwidth and pairing interactions, reinforcing the importance of precise oxygen control for achieving high-performance HTS materials.

6.3 Structural Anisotropy and Current Transport Properties

The intrinsically layered nature of HTS materials gives rise to pronounced anisotropy in electrical transport behavior. Experimental results consistently show that the critical current density (Jc) is substantially higher within the CuO_2 planes than along the crystallographic c-axis. Investigations of grain boundary effects further reveal that misorientation angles beyond a critical value cause an exponential reduction in Jc, highlighting the sensitivity of current transport to structural alignment (Hilgenkamp &Mannhart, 2002).

These findings help explain the difficulties encountered in fabricating polycrystalline HTS conductors and emphasize the need for processing techniques that promote strong crystallographic texture and grain alignment.

6.4 Influence of Defects and Lattice Strain

Defects and lattice strain are found to play a dual role in high-temperature superconductors. While excessive disorder generally degrades superconducting properties, the controlled introduction of defects can enhance flux pinning and improve performance under applied magnetic fields. The analysis suggests that

nanoscale structural inhomogeneities, when carefully engineered, can contribute positively to superconducting functionality without causing a significant reduction in Tc (Blatter et al., 1994).

Taken together, these results demonstrate that superconducting behavior in high-temperature superconductors is governed by a delicate balance among multiple structural factors. Layered architecture, oxygen stoichiometry, lattice symmetry, and defect distribution collectively determine overall superconducting performance. These findings strongly support the central conclusion that targeted structural optimization is a key strategy for advancing the development of high-temperature superconducting materials.

VII. Conclusion

This study has provided a detailed examination of the structure–property relationship in high-temperature superconducting materials, with a particular focus on cuprate-based superconductors. The analysis clearly shows that superconducting behavior in these materials is fundamentally governed by their complex crystal structures. Structural features such as the presence of layered CuO_2 planes, oxygen stoichiometry, lattice distortions, and anisotropy collectively control key superconducting parameters, including the critical temperature, critical current density, and magnetic field response.

The results confirm that superconductivity in high-temperature superconductors is largely confined to the quasi-two-dimensional CuO_2 planes, where strong electronic correlations and orbital hybridization play a dominant role. Precise regulation of oxygen content emerges as a crucial factor for optimizing charge carrier concentration and achieving maximum critical temperature. In addition, improved lattice symmetry and reduced structural distortion are shown to favor enhanced superconducting performance. At the same time, pronounced structural anisotropy and weak intergranular coupling continue to pose significant challenges for large-scale and practical applications.

Overall, this work reinforces the view that high-temperature superconductivity cannot be fully understood without careful consideration of crystal structure. The strong sensitivity of superconducting properties to even subtle structural variations highlights the importance of precise structural engineering and the use of advanced characterization techniques. The insights gained from this study provide a strong foundation for future research aimed at improving both the performance and practical applicability of high-temperature superconducting materials.

VIII. Future Scope

Despite the considerable progress made in understanding high-temperature superconducting materials, substantial opportunities remain for future research and technological advancement. Further development in this field will require a multidisciplinary approach that brings together materials science, condensed matter physics, chemistry, and computational modeling. One of the most promising directions for future work involves achieving precise control over crystal structure at the atomic scale. Advanced synthesis techniques, such as molecular beam epitaxy, pulsed laser deposition, and atomic-layer engineering, offer the ability to fabricate highly ordered superconducting structures with tailored properties. These approaches provide opportunities to systematically tune interlayer spacing, lattice strain, and defect distribution, which may lead to further improvements in critical temperature and current-carrying capacity.

Another important avenue for future investigation is the exploration of superconducting material families beyond conventional cuprates. Although iron-based and nickel-based superconductors have already broadened the scope of high-temperature superconductivity, continued research into novel layered compounds, interfaces, and heterostructures may yield materials with higher transition temperatures or improved mechanical robustness. Such discoveries could significantly enhance the practical applicability of superconducting technologies.

Theoretical modeling also remains a crucial area for future progress. Developing comprehensive theoretical frameworks that simultaneously account for strong electronic correlations, lattice effects, and magnetic interactions continues to be a major challenge. Advances in computational techniques, including density functional theory combined with many-body and beyond-mean-field approaches, are expected to provide deeper insight into the microscopic mechanisms of superconductivity. These developments may ultimately enable more reliable, predictive strategies for the design of new superconducting materials.

From an application-oriented perspective, future research must also address challenges related to scalability and cost. Improvements in fabrication techniques for superconducting wires, tapes, and bulk components, along with more effective flux pinning strategies, are essential for large-scale implementation. Progress in these areas is particularly important for applications such as power transmission, magnetic levitation, and energy storage systems. Overall, continued investigation of structure–property relationships, supported by technological innovation and theoretical advancement, has the potential to unlock the full capabilities of high-temperature superconducting materials and extend their impact across a wide range of scientific and industrial domains.

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