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FUNCTIONAL PROPERTIES OF BOROPHENE-BASED MATERIALS: STRUCTURE–PROPERTY–APPLICATION RELATIONSHIP

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Abstract

This study examines the relationship between the structural properties and functional performance of borophene-based materials from a holistic perspective. Borophene, as a next-generation two-dimensional material, exhibits remarkable properties such as high mechanical strength, superior electrical conductivity, and high thermal conductivity due to its atomically thin structure, three-center bonding mechanism, and vacancy-rich crystal lattice.

In this work, the crystal structure, chemical composition, and synthesis methods of borophene are analyzed in detail, and the effects of these structural parameters on its mechanical, electronic, and thermal properties are systematically evaluated. Furthermore, the impact of different production techniques (such as MBE, CVD, and exfoliation methods) on material performance is emphasized. The study also highlights the critical role of defect engineering and chemical doping in optimizing borophene's functional properties.

The findings demonstrate that borophene is not a material with fixed properties; rather, it serves as an adaptable engineering platform whose characteristics can be tailored depending on the application through structure–property relationships. Finally, the application potential of borophene in fields such as energy storage, nanoelectronics, aerospace, and sensor technologies is discussed. However, challenges such as large-scale production, high cost, and structural stability must be addressed. This study aims to provide a systematic framework for future research by offering a comprehensive perspective on borophene.

Keywords: Borophene, two-dimensional materials, structure–property relationship, mechanical properties, electronic properties, thermal conductivity, defect engineering, chemical doping, energy storage, nanoelectronics

1. Introduction

The performance criteria expected from materials used in advanced engineering applications have undergone significant changes in recent years, necessitating a departure from the classical material paradigm. In particular, the simultaneous achievement of high strength and low density in fields such as aerospace, energy storage, and nanoelectronics has directed materials science research toward two-dimensional (2D) materials. In this context, among the new generation of atomically layered structures developed in the post-graphene era, borophene has attracted considerable attention due to its unique mechanical and physical properties.

Borophene is the single-atom-thick crystalline form of the natural element boron and stands out with its high mechanical strength, exceptional flexibility, and high thermal conductivity [2]. Initially predicted theoretically, this structure was experimentally synthesized in 2015, marking a significant contribution to the family of two-dimensional materials [6]. This development led to a rapid increase in studies focusing on borophene, and its electronic, optical, and mechanical properties have since been extensively investigated. The fact that borophene exhibits higher strength and flexibility potential compared to graphene places it in a more advantageous position for advanced engineering applications [7, 11].

One of the most remarkable features of borophene is that, unlike conventional two-dimensional materials, it possesses a vacancy-rich crystal structure and a three-center bonding mechanism. This bonding configuration enables the material to exhibit both high strength and flexibility while also giving rise to direction-dependent (anisotropic) physical properties [12]. This indicates that the properties of borophene are strongly dependent not only on its chemical composition but also on its atomic arrangement and synthesis conditions.

The production methods of borophene constitute another critical parameter that directly affects its structural and functional properties. Borophene structures synthesized via techniques such as molecular beam epitaxy (MBE) and chemical vapor deposition (CVD) differ in terms of crystal quality, defect density, and homogeneity, which in turn significantly influence their mechanical and electronic performance [6, 10]. In addition, alternative production techniques such as liquid-phase exfoliation and sonochemical methods offer advantages in terms of cost and scalability; however, they also present certain limitations in structural control.

From the perspective of functional properties, borophene stands out as a versatile material due to its high elastic modulus, excellent electrical conductivity, and high thermal conductivity. The literature reports that the elastic modulus of borophene can reach approximately 210 N/m, which is considerably higher than that of many conventional materials [9]. Furthermore, its high carrier mobility and tunable band structure make borophene a strong candidate for nanoelectronic applications [7].

Although a significant portion of the studies on borophene has focused on investigating its individual properties, research addressing the relationship between these properties and atomic structure and synthesis parameters in a holistic manner remains limited. However, in order to fully reveal the practical application potential of borophene, it is essential to systematically analyze the structure–property–application relationship. In this context, understanding how the mechanical, electronic, and thermal properties arising from the atomic structure of borophene are influenced by different production methods and chemical modifications is of critical importance.

This study aims to comprehensively examine the relationship between the structural characteristics and functional performance of borophene-based materials. Within this scope, the crystal structure, chemical modifications, and synthesis methods of borophene are discussed, followed by an evaluation of how these structural parameters affect its mechanical, electronic, and thermal properties. Finally, potential applications of borophene in fields such as energy, aerospace, and nanoelectronics are assessed within the framework of the structure–property relationship. This approach aims to provide a holistic perspective to the borophene literature and to establish a guiding framework for future research.

2. Structural Properties of Borophene-Based Materials

To understand the functional performance of borophene, it is necessary to holistically consider the relationship between its atomic structure, chemical composition, and synthesis methods. Unlike other two-dimensional materials, borophene exhibits a structurally flexible and polymorphic character, which directly influences its functional properties.

2.1. Crystal Structure and Atomic Arrangement of Borophene

Although borophene is a two-dimensional crystalline structure composed of boron atoms, it does not possess a fully filled hexagonal lattice like graphene. Instead, it exhibits a complex lattice structure containing vacancies in specific proportions to compensate for electron deficiency. This vacancy-rich structure not only ensures the thermodynamic stability of borophene but also emerges as a key parameter directly determining its mechanical and electronic properties [12].

The most distinctive structural feature of borophene is its three-center bonding mechanism. Unlike conventional two-center covalent bonds, this type of bonding allows electrons to be shared among multiple atoms, thereby enabling both high mechanical strength and flexibility. As a result, borophene is not only a strong material but also highly resistant to deformation.

In addition, borophene exhibits structural anisotropy. Significant variations in mechanical and electronic properties are observed depending on the crystal orientation. This direction-dependent behavior is considered a critical design parameter, particularly in applications involving mechanical loading and electronic transport.

In this context, the atomic arrangement of borophene should be regarded not merely as a static feature but as a dynamic parameter that determines its functional performance.

2.2. Chemical Composition and Derivatives

Borophene offers a wide range of applications due to its chemically modifiable nature. Its fundamental structure, composed of pure boron atoms, can be significantly altered through doping with different elements or surface functionalization.

The literature reports various derivatives of borophene, such as B-borophene, O-borophene, N-borophene, and F-borophene [2]. These derivatives are obtained either by partially substituting boron atoms with other elements or through surface modification.

Such chemical modifications directly affect the electronic structure and surface properties of borophene. For instance, oxygen-doped borophene structures have been reported to exhibit enhanced electrical conductivity, whereas nitrogen-doped structures demonstrate superior catalytic activity [12]. This versatility allows borophene to be tailored as an “engineering material” for application-specific requirements.

However, it should be noted that chemical modifications not only provide advantages but may also introduce new challenges, such as reduced structural stability and increased synthesis complexity. Therefore, studies on borophene derivatives should focus not only on performance enhancement but also on stability and manufacturability criteria.

2.3. Synthesis Methods and Their Structural Effects

The synthesis methods of borophene play a decisive role in determining its structural integrity, defect density, and consequently its functional properties. Various synthesis techniques have been developed, each with its own advantages and limitations.

Molecular beam epitaxy (MBE) is considered one of the most effective methods for producing high-purity borophene with well-ordered crystal structures. However, it suffers from disadvantages such as high cost and low production rates. In contrast, chemical vapor deposition (CVD) offers a more economical alternative, although the resulting borophene structures generally exhibit lower crystal quality [6, 10].

Alternatively, liquid-phase exfoliation (LPE) and sonochemical methods reduce production costs and provide advantages in terms of scalability. However, these methods face significant challenges in controlling the size and achieving homogeneity of borophene layers [1, 4].

The comparative analysis presented in the referenced book section (Table 2) clearly highlights the advantages and disadvantages of these synthesis methods.

For example, while MBE offers high quality, it is cost-intensive; conversely, sonochemical methods are more economical but limited in terms of quality and structural control.

In this regard, the selection of a synthesis method should be considered not only an economic decision but also a performance-oriented one. Particularly in advanced engineering applications, where high performance is required, the influence of the synthesis method on the microstructure becomes a critical design parameter.

In conclusion, the structural properties of borophene arise from complex interactions between atomic arrangement, chemical composition, and synthesis methods. Understanding these interactions is essential for accurately establishing the structure–property relationship.

Table 1. Comparative evaluation of borophene production techniques [1, 4, 6, 10].

Production Technique	**Structural Quality**	**Scalability**	**Cost Level**	**Structural Control**	**Main Advantage**	**Primary Limitation**
Molecular Beam Epitaxy (MBE)	Very High	Low	High	Very Precise	Atomic-level crystal quality	Not suitable for industrial production
Chemical Vapor Deposition (CVD)	Medium–High	Medium	Medium	Good	Larger-area production capability	Risk of defect formation
Liquid Phase Exfoliation (LPE)	Medium	High	Low	Limited	Economical and scalable	Difficult control of size and thickness
Sonochemical Method	Medium	High	Low	Limited	Simple and rapid production	Low structural homogeneity
Molten Salt Method	Medium–High	Medium	Medium	Developing	Novel generation production approach	Insufficient literature availability

This table not only highlights the technical differences among borophene production methods but also reveals their impact on the structure property relationship. While the MBE method stands out in applications requiring high crystal quality, CVD and exfoliation-based techniques appear more suitable for applications that demand large surface areas, such as energy storage and coating technologies. This indicates that the production method is not merely a synthesis parameter but also a critical design variable that determines the final application performance.

3. Functional Properties: Mechanical, Electronic, and Thermal Behavior

The functional properties of borophene arise directly from its atomic structure and bonding characteristics, and these properties determine its performance across various engineering applications. In this section, the mechanical, electronic, and thermal properties of borophene are not only described but also analyzed in terms of their underlying mechanisms and compared with other two-dimensional materials.

3.1. Mechanical Properties and Strength Mechanisms

Borophene stands out among two-dimensional materials due to its exceptionally high mechanical strength. The literature reports that the elastic modulus of borophene can reach approximately 210 N/m. This value is considerably higher than that of many conventional engineering materials and, when combined with its low density, provides borophene with superior specific strength.

The primary reason for this high strength lies in the three-center bonding mechanism between boron atoms. Compared to classical two-center covalent bonds, this bonding configuration enables a more flexible distribution of electrons, allowing the material to exhibit both high strength and significant deformation capability.

However, borophene demonstrates more complex mechanical behavior compared to graphene. While graphene exhibits isotropic properties, borophene has an anisotropic structure. This leads to variations in mechanical properties depending on the crystal orientation [12]. For example, higher elastic modulus and tensile strength may be observed in certain directions, whereas greater flexibility may be present in others.

In addition, borophene's high fracture toughness and its ability to recover after deformation make it suitable for systems subjected to dynamic loading. These properties provide a critical advantage, particularly in aerospace applications, where there is a strong demand for lightweight materials with high impact resistance.

3.2. Electrical and Electronic Properties

Borophene occupies a unique position among two-dimensional materials in terms of its electronic properties. Unlike materials such as graphene, which possess a zero band gap, the electronic structure of borophene can vary depending on synthesis conditions and crystal phase.

One of the most significant characteristics of borophene is its ability to exhibit metallic conductivity. When combined with high carrier density and mobility, this makes borophene a strong candidate for high-speed electronic devices [7].

Furthermore, the band structure of borophene can be tuned through chemical doping or structural modifications. This feature enables its use in both conductive and semiconductive applications. Such tunable electronic properties are particularly important for nanoelectronic and flexible electronic systems.

Another remarkable property of borophene is its ability to exhibit superconducting behavior under certain conditions. This suggests that borophene is not only suitable for conventional electronic applications but also holds potential for quantum technologies.

3.3. Thermal Conductivity and Heat Management

Borophene offers a significant advantage in systems requiring efficient heat management due to its high thermal conductivity. Effective dissipation of heat generated in electronic devices is a critical parameter for both performance and reliability.

The high thermal conductivity of borophene is associated with efficient phonon transport. Its well-ordered atomic structure and strong bonding characteristics enable rapid transfer of thermal energy [11].

This property makes borophene a promising candidate for high-performance microelectronic systems and thermal management applications. Additionally, in aerospace applications, the use of borophene in components exposed to high temperature gradients may enhance overall system stability.

3.4. Surface Properties and Chemical Reactivity

The high surface area and chemical reactivity of borophene make it extremely valuable for catalytic and sensor applications. Due to its atomically thin structure, a large proportion of its surface atoms remain active, which enhances reaction kinetics.

Borophene has been reported to exhibit high sensitivity, particularly in gas sensing applications. This behavior is closely related to the efficiency of adsorption processes occurring on its surface [8]. Moreover, the catalytic properties of borophene provide significant advantages in energy conversion reactions, such as hydrogen production.

These features position borophene not only as a structural material but also as a highly functional surface material.

4. Structure–Property Relationship and Performance Analysis

The functional performance of borophene-based materials arises from complex interactions among atomic structure, chemical composition, and synthesis parameters. In this context, the structure property relationship is one of the most critical aspects to be understood, not only from a fundamental science perspective but also for engineering applications. Although numerous studies in the literature focus on the individual properties of borophene, comprehensive analyses directly correlating these properties with structural parameters remain limited. Therefore, identifying the fundamental mechanisms that determine the performance of borophene is of great importance.

4.1. Effect of Atomic Structure on Functional Properties

The vacancy-rich crystal structure of borophene at the atomic level, along with its three-center bonding mechanism, directly determines its mechanical, electronic, and thermal properties. In particular, the vacancy concentration emerges as a key parameter influencing both the strength and conductivity of the material.

Structures with low vacancy concentration exhibit higher mechanical strength, whereas increasing vacancy concentration enhances flexibility and deformation capability. This indicates that borophene can be optimized depending on the intended application. For example, denser crystal structures are preferred in structural applications requiring high strength, while structures with higher vacancy concentration may provide advantages in electronic applications requiring flexibility [12].

In addition, the anisotropic nature of borophene causes its properties to vary depending on direction. This direction-dependent behavior should be considered a critical design parameter, particularly in applications involving mechanical loading and electrical conduction.

4.2. Correlation Between Synthesis Method and Performance

The synthesis methods of borophene directly influence its microstructure and, consequently, its macroscopic performance. Borophene structures produced via molecular beam epitaxy (MBE) exhibit superior mechanical and electronic properties due to their low defect density and high crystal order. In contrast, structures obtained through more economical methods such as chemical vapor deposition (CVD) or exfoliation techniques tend to contain higher defect densities, which may lead to reduced performance [6].

In this context, it should also be recognized that defects are not solely detrimental but can, in certain cases, provide functional advantages. For example, the controlled introduction of defects may enhance the catalytic activity of borophene or improve its surface reactivity. Therefore, the selection of a synthesis method should not be based solely on cost considerations but also on performance criteria aligned with the intended application. This approach enables borophene to be evaluated within the framework of "application-specific material design."

4.3. Defects, Doping, and Property Engineering

One of the most important approaches for optimizing the functional properties of borophene is defect engineering and chemical doping. Defects introduced at the atomic scale can alter the electronic structure of the material, directly affecting properties such as conductivity, catalytic activity, and energy storage capacity.

In particular, doping processes enable the customization of borophene according to specific applications. For instance, studies on hydrogen storage applications have shown that borophene structures doped with certain metal atoms exhibit high capacity and stability [5]. Similarly, nitrogen- or oxygen-doped structures can demonstrate enhanced activity in catalytic reactions.

However, uncontrolled implementation of defect creation and doping may negatively affect structural stability and lead to a decrease in mechanical strength. Therefore, property engineering in borophene-based materials should be treated as an optimization problem requiring a careful balance.

In this regard, borophene can be considered not only a material with intrinsic properties but also a "smart material platform" that can be optimized through engineering interventions.

Table 2. The effect of structural parameters on functional properties and performance in borophene [7, 8, 9, 12].

Structural Parameter	Microstructural Effect	Effect on Functional Properties	Performance Outcome / Application Implication
Vacancy concentration	Reduction in crystal continuity	Elasticity ↑, strength ↓ (at high levels)	Flexible electronics, sensor applications
Three-center bonding structure	Electron delocalization	High mechanical strength and flexibility	Lightweight and durable structural materials
Crystal orientation (anisotropy)	Direction-dependent bonding distribution	Directional variation in mechanical and electronic properties	Design of direction-controlled devices
Defect density	Increase in local irregularities	Conductivity ↓, catalytic activity ↑	Catalysis and energy conversion systems
Doping (O, N, F, etc.)	Modification of electronic structure	Tunable conductivity and reactivity	Sensors, battery electrodes
Synthesis method (MBE, CVD, etc.)	Crystal quality and homogeneity	Variation in mechanical and electronic performance	High-performance or cost-effective applications

As shown in Table 2, the functional properties of borophene are directly dependent on its structural parameters, and this relationship has been extensively discussed in the literature [2]. In particular, parameters such as vacancy concentration, defect density, and doping play a decisive role in determining the material's mechanical strength, electrical conductivity, and chemical reactivity. This indicates that, rather than being a material with fixed properties, borophene offers a structure that can be optimized for specific applications.

For example, while low defect density and high crystal order are preferred in applications requiring high strength, controlled defect introduction and doping processes can enhance performance in catalytic or sensor applications. In this context, the structure–property relationship of borophene should be considered not as a one-dimensional correlation, as in classical materials, but as a multi-parameter and optimizable system.

5. Application Areas and Technological Potential

Borophene addresses a wide range of applications due to its superior mechanical, electronic, and thermal properties. However, evaluating these applications requires not only listing these properties but also analyzing how they align with specific engineering requirements. In this context, the application potential of borophene should be considered from a structure–property relationship perspective.

5.1. Energy Storage and Conversion Systems

One of the most prominent application areas of borophene is energy storage systems. In particular, its use as an anode material in lithium-ion batteries offers significant advantages due to its high theoretical capacity and fast ion diffusion characteristics. The literature indicates that borophene can achieve much higher capacity values compared to conventional graphite anodes [3].

This performance is primarily attributed to borophene’s high surface area and the presence of vacancies in its atomic structure, which are favorable for ion storage. Additionally, it has been demonstrated that this capacity can be further enhanced through doping and surface modification.

However, one of the major limitations of borophene in energy applications is related to production scalability and stability issues. In particular, further research is needed to improve long cycle life and structural stability.

5.2. Electronic and Nanoelectronic Applications

Borophene is a promising candidate for nanoelectronic applications due to its high carrier mobility and metallic conductivity. In flexible electronic systems, its combination of mechanical flexibility and electrical performance provides significant advantages.

The tunability of borophene’s band structure makes it suitable not only for conductive applications but also for semiconducting ones. This enhances its potential use in areas such as transistors, sensors, and flexible display technologies [7].

However, a critical limitation in this field is that large-scale and defect-free production of borophene is not yet feasible. Since defect control is essential for high performance in electronic applications, further development of synthesis techniques is required.

5.3. Aerospace Materials

The combination of low density and high mechanical strength makes borophene an extremely attractive material for aerospace applications. The use of lightweight and durable materials is crucial for fuel efficiency and overall system performance.

When used as a reinforcement element in composite materials, borophene can increase mechanical strength while reducing overall weight. Moreover, its high thermal conductivity can improve heat management in systems exposed to high temperature gradients.

Nevertheless, the application of borophene in aerospace is still at an early stage. Further research is required, particularly in areas such as large-scale production and long-term environmental durability.

5.4. Biomedical and Sensor Technologies

The high surface reactivity and large surface area of borophene make it suitable for biomedical and sensor applications. Its high sensitivity in gas sensing applications provides a significant advantage for environmental monitoring and healthcare technologies [12].

Additionally, if borophene can be rendered biocompatible, it may be utilized in areas such as drug delivery systems and biosensors. However, issues such as toxicity and biological interactions must be thoroughly investigated for such applications.

In this context, although borophene holds significant potential in biomedical applications, it can still be considered to be in the early stages of research.

Table 3. Relationship between the functional properties of borophene and its application areas [3, 7, 8].

Functional Property	Provided Advantage	Application Area	Critical Limitation
High surface area	High ion storage capacity	Batteries, supercapacitors	Structural stability
Metallic conductivity	Fast electron transport	Nanoelectronic devices	Sensitivity to defects
High mechanical strength	Lightweight and durable structure	Aerospace composites	Scalable production
High thermal conductivity	Efficient heat dissipation	Microelectronic systems	Integration challenges
Chemical reactivity	High sensor sensitivity	Gas sensors, catalysis	Stability

Table 3 illustrates the direct relationship between the functional properties of borophene and its application areas. As observed, each property provides advantages in specific applications while also involving certain limitations. This indicates that the application performance of borophene depends not only on its intrinsic properties but also on how effectively these properties are optimized. Therefore, rather than being a material with fixed characteristics, borophene should be considered a platform that can be tailored through engineering interventions according to specific application requirements.

6. Conclusion

This study expands upon previously presented borophene-based analyses by addressing the structure–property–application relationship within a more comprehensive framework [2]. The findings clearly demonstrate that the mechanical, electronic, and thermal properties of borophene are directly related to its atomic structure, bonding characteristics, and synthesis parameters. In particular, distinctive features such as three-center bonding, a vacancy-rich crystal lattice, and anisotropic structure emerge as the key factors that differentiate borophene from other two-dimensional materials.

From a structure–property perspective, borophene cannot be considered a material with fixed characteristics; rather, it represents an "engineering platform" that can be optimized through synthesis methods, defect density control, and chemical modifications. This adaptability enables borophene to be tailored for various applications, making it a highly flexible candidate for advanced engineering systems.

In terms of functional properties, borophene offers versatile advantages, including high mechanical strength, excellent electrical conductivity, and high thermal conductivity. These properties highlight its potential across a broad range of applications, from energy storage systems and nanoelectronic devices to aerospace structures and sensor technologies. However, the full realization of this potential depends on a deeper understanding of structure–property relationships and the advancement of synthesis techniques.

One of the major barriers to the industrial integration of borophene is related to large-scale production challenges, high cost, and structural stability issues. In particular, the limited availability of high-crystal-quality borophene directly affects its performance in electronic and mechanical applications. Therefore, future research should focus on developing scalable production methods and optimizing defect control.

In addition, defect engineering and doping strategies play a critical role in tuning the functional properties of borophene for specific applications. However, the impact of such modifications on structural stability requires further detailed investigation. In this regard, combining multiscale modeling approaches with experimental studies will contribute significantly to a better understanding of borophene behavior.

From a future perspective, borophene is expected to play a significant role not only in current applications but also in next-generation technologies. In particular, hydrogen storage systems, flexible electronics, quantum devices, and high-performance composite materials are among the areas where borophene may have transformative potential. Nevertheless, realizing this potential will require increased interdisciplinary collaboration and stronger integration between fundamental science and engineering applications.

In conclusion, due to its unique structure–property relationship, borophene should be regarded not only as a new research topic in materials science but also as a strategic material candidate for future high-performance engineering systems. The holistic approach presented in this study is expected to contribute to the borophene literature and provide a guiding framework for future research.

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