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Atmospheric Stability of Two-Dimensional Black Phosphorus and the Role of h-BN Encapsulation

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Abstract. Black Phosphorus (BP) is a layered semiconductor. It has a tunable band gap, high carrier mobility and strong in-plane aisotropy, with a wide optical response. However, its application is limited by the rapid degradation of the ambient environment, where the oxidation of oxygen, water and light promotes surface oxidation, and also damages the electronic and optical properties. This study explores the atmospheric degradation situation of Two-Dimensional(2D) BP, as well as the protective effect of Hexagonal boron oxide nitride(h-BN) encapsulation. Analyze the degradation mechanisms of BP in oxygen, water, and illumination, focusing on the synergistic effect of environmental factors and surface defects. Evaluate the protection mechanism of h-B encapsulation, such as the physical barrier between oxygen and water and the van der Waals interaction with BP. Evaluate the impact of h-B encapsulation on the structure, electrical and optical properties of BP, and compare it with the traditional oxide and polymer protection layer. Finally, discuss its limitations, such as defects, edge exposures, transfer residues and fabrication scalability. These results show that the encapsulation of h-BN is an effective way to improve the environmental stability and intrinsic properties of BP devices.

Keywords: Black phosphorus; H-BN encapsulation; Atmospheric stability; Degradation; Van der Waals interface.

1. Introduction

BP is a two-dimensional black phosphorus semiconductor, which has a tunable band gap, high carrier mobility, good in-plane aisotropy and broad optical response in the infrared region. These characteristics make BP a promising material for applications in field effect transistors, photodetsectors and other electronic/optical devices [1-3]. In particular, BP has the characteristics of thickness and strong optical response, which distinguishes it from other widely studied two-dimensional materials such as graphene and transition metals.

BP has anisotropic crystal structures. Its puckered structure has different physical properties in the armchair and the zigzag direction, which leads to the transport of charge and optical response [1,3]. As shown in Figure 1, AC and zigzag directions come from the puckered phosphorene structure. BP bandgap can be adjusted by changing thickness, providing a certain degree of freedom for nanoscale electronic devices. These characteristics make BP an attractive candidate in applications that require electrical transmission and optical sensitivity.

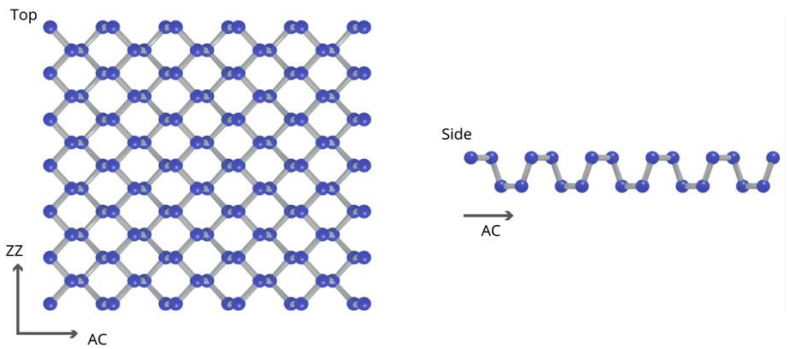

Figure 1. Top and bottom views of the monolayer phosphorene structure, with the armchair and zigzag directions indicated [4].

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BP has advantages, but its practical application is limited by poor stability in the ambient environment. Previous research has shown that BP will degrade rapidly when exposed to oxygen, moisture and light, and the structure and electronic properties will change [5-8]. Oxygen is the main factor in degradation, and water will have an impact on reaction environment and degradation. Illumination can accelerate degradation by photooxidation [6]. Therefore, improving BP's environmental stability is a key requirement for reliable BP-based devices.

BP degradation is particularly problematic in ultrathin samples, because a large amount of the material is close to the surface. Surface oxidation will cause defects and modify BP electronic structure, which will also affect carrier transportation and device performance [8-9]. So environmental protection is not just a matter of materials stability, but also related to the long-term reliability of BP electronic devices.

Several protection strategies are developed to improve BP stability, such as polymer coatings, O-layer deposition of oxide films and encapsulation of other two-dimensional materials [8]. Hexagonal h-B has attracted attention because it has high chemical properties, is flat on the surface, has electrical insulation, and is compatible with van der Waal heterostructures [10-13]. H-BN has a clean interface with BP, and there is no traditional covalent bond between the two materials.

This article analyzes the atmospheric degradation of BP, and also evaluates the role of the encapsulation of h-BN in improving environmental stability. Discuss the physical barrier effect and the Van der Waals interface, then analyze the impact of encapsulating on BP intrinsic properties. Finally, compare the encapsulation of h-BN with traditional oxide and polymer protection strategies, and discuss the current limitations and future directions.

2. Atmospheric Degradation of Black Phosphorus

BP is affected by the interaction of oxygen, water and light [5-8]. The chemical active phosphorus atoms on the surface of BP make the material vulnerable to atmospheric species reactions. Due to the high surface-volume ratio of low-layer and ultra-thick BP, this problem is relatively important.

Experiments and theoretical studies show that oxygen plays a major role in BP degradation. Oxygen molecules interact with phosphorus atoms at the BP surface, initiate oxidation reactions, and form phosphorus-oxygen-related species. Hang et al. found that oxygen undergoes dissociation chemisorption of BP, and the presence of water will affect the degradation environment [6]. The results show that O is the key factor in BP deterioration, not just water as the main oxidizing factor.

Water is an important environmental factor, and its effect depends on the chemical conditions and oxygen availability [6]. Therefore, controlling oxygen and moisture is very important for BP's atmospheric stability.

Light is another key path for accelerated degradation. Favron et al. pointed out that light can accelerate the photooxygenation of exfoliated blood BP [7]. Light interacts with BP, generating photoexcited carriers and participating in surface reactions with oxygen and other atmospheric substances. So BP may degrade more rapidly under light than under dark conditions [7]. This phenomenon is related to the BP photodetector, because light exposure is a key part of normal operation.

After atmospheric degradation, oxidized areas and structural defects develop on the surface of the BP [5–8]. These changes can change the local electronic structure, and also increase the disorder in the material. In ultrathin oil, surface degradation has a strong impact, because the surface is a large amount of active material.

The environmental instability of BP is a combination of chemical and physical problems. Atmospheric molecules first interact with the surface of the exposed BP, then undergo oxidation, defect formation and modification of electronic properties [5-7]. Effective protection needs to reduce the flow of oxygen/methane to BP and avoid significant damage to the crystal structure/electronic properties [5,11,12].

These degradation processes will have an impact on BP-based devices' performance and reliability. Surface oxidation or defect formation will introduce additional electronic states, increase carrier scattering, and reduce carrier transport efficiency [5,8]. BP field-effect transistors (FETs) need high carrier mobility and a stable threshold voltage to operate reliably.

The research results of Wood et al. show that ambient exposure can greatly reduce the performance of BP transistor [8]. In the unprotected BP FET, the threshold voltage changes significantly during atmospheric exposure; prolonged exposure will cause about three orders of magnitude of changes in mobility and current off/off ratio. Observations show that atmospheric degradation can quickly transform high-performance BP transistors into less effective devices.

In terms of long-term reliability, Illarionov and others studied BP FETs, and found that environmental degradation will affect the electrical properties of the device over time [9]. Changes in carrier transportation, threshold voltage and other transistor parameters will reduce the reproducibility of BP circuits and limit the actual lifetime of the BP circuit.

Degravation has an impact on optoelectronic equipment. BP has strong infrared response, which is attractive to infrared photodetector [1,3]. But surface oxidation and photo-induced degradation will interfere with photoexcited carriers' generation, recombination and transport. This will reduce photoresponse, and also affect the stability of long-term devices.

Observations show that preventing BP from entering the atmosphere is very important for material quality and device function. Effective encapsulation methods need to ensure strong environmental protection and do not introduce additional electrical, chemical and structural disturbances.

3. Properties of h-BN Relevant to Encapsulation

H-BN is layered two-dimensional materials with a crystal structure like that of graphite, and the boron and nitrogen atoms are in the hexagonal honeycomb layer in each layer. There is strong covalent bonding between the atoms of the same layer, and adjacent layers are mainly connected through weak Van der Waals interaction. This layered structure can be used to prepare thin H-BN flakes by mechanical exfoliation or other methods.

H-BN has several properties that make it attractive for BP encapsulation. First, its chemical stability and thermal stability are relatively high [11-13]. The protective material is stable under environmental conditions, and is not a major source of chemical pollution.

Second, the atomically flat surface of h-B is important for two-dimensional heterostructures. Interface roughness and disorder will affect carrier transport. A flat H-BN surface provides a relatively clean interface compared with some traditional deposited films.

Third, h-B is a wide-bandgap electrical insulator [11-13]. It can protect the BP channel, and is not a traditional conducting layer. This is useful for electronic devices, because the protective layer does not introduce unwanted electrical conduction paths.

The layered structure of h-BN enables van der Waals to interface with BP. Strong covalent bonds between the two materials are not needed, which can reduce BP surface chemical modification during encapsulation. Two-dimensional materials have electronic properties that are highly sensitive to surfaces. H-BN has chemical stability and atomic flatness, has electrical insulation, and is compatible with van der Waals, making it a promising material for BP to resist atmospheric degradation [11-13].

4. Protection Mechanisms of h-BN Encapsulation

4.1. Physical Barrier Effect

H-BN encapsulation has a physical barrier effect. The BP layer is between two h-B layers. The encapsulating layer reduces the direct exposure to BP by atmospheric oxygen and moisture [11,12].

A continuous high-quality H-BN layer can reduce the probability of reactive atmospheric species reaching the BP surface. This can suppress surface oxidation rate and extend the operational life of BP devices [11,12]. Experimental studies show that fully encapsulating BP FETs have better air stability than unprotected devices [11,12].

The top H-BN layer can reduce the direct BP exposure to the surrounding environment, and also modify the active layer optical environment. This may be beneficial, because illumination can accelerate the photooxidation of BP [7]. But h-BN is not an absolute barrier to all environmental impacts. The encapsulation effect depends on the continuity or quality of the h -BN layer.

Defects such as cracks, bubbles, uncovered edges or contamination during transfer may create pathways for oxygen and moisture to reach BP. So the quality of encapsulation structure is the key to its long-term effect.

Sar et al. showed that the air-stable transport of graphene-contacted fully encapsulated ultra-thin BP FETs was achieved, providing experimental evidence for the effect of H-BN encapsulation [9]. More recent studies have further demonstrated the stability and stability of full-encapsulated BP ETSs, and also emphasized the importance of encapsulating structure in device performance [12].

4.2. Van Der Waals Interface

H-BN encapsulation has the advantage of van der Waals interfaces [9-13]. Unlike traditional deposited protective films, it does not need a strong covalent bond with BP. The two materials are stacked through weak interlayer interaction.

This interface can reduce lattice matching and reduce the chemical reactions between encapsulation layer and BP surface [9,12]. These characteristics are very valuable for two-dimensional materials, because their electronic properties are strongly affected by surface chemistry and interfaces.

Van der Waals interface can construct atomically thin nanostructures without greatly increasing the thickness of overall devices. This is advantageous in nanoscale electronic/optoelectronic applications, where the active structure is relatively thin.

Birowka et al. studied the impact of h-B encapsulation on the structure and vibration properties of few-layer BP, and found that it can change the physical environment and structure of BP while maintaining the overall layered structure [13]. Therefore, it not only acts as a protective barrier, but also provides a clean platform for studying BP in the van der Waals structure.

4.3. Influence of Encapsulation on the Intrinsic Properties of BP

H-BN encapsulation has a certain degree of protection, but it is not completely free of disturbances. The introduction of H-B changes the environment of BP and may also affect the electronic and optical properties of the device.

For example, the interface charge and the dielectric screening of BP can change the electrostatic environment. Two-dimensional materials have electronic and optical properties that can be sensitive to the diode environment, and h-BN may affect properties such as carrier interaction, optical transition and so on.

Mechanical effects need to be considered. Local strains, thermal expansion differences, and imperfections in stacking will affect the BP level. The trapped bubbles or transfer residues may cause local changes in the interface and also lead to device-device interface differences.

Therefore, h-B is a low-disturbance encapsulation strategy, not a completely disturbance-free method. The goal is to reduce the impact of encapsulating and improve environmental stability.

The balance between protection and intrinsic properties is the key to the attractiveness of h-BN for BP devices. The encapsulation layer needs to be effective to prevent degradation and be clean and chemically stable, so as not to introduce new defects.

5. Comparison with Conventional Encapsulation Strategies

5.1. Atomic Layer Deposition of Oxides

In addition to H-BN, ALD is used to protect BP from environmental degradation [8,10]. AlD can control the thickness of film, and can also produce conformal coating, which is attractive for large-scale device manufacturing.

Oxide layers are effective in protecting oxygen and moisture. Wood et al. pointed out that ALD passivation can improve BP transistors' environmental stability [8]. Oxygen encapsulation has potential in device manufacturing.

Aluminum hydroxide (ALD) deposition has chemical differences compared with h-B encapsulation. ALD involves the reaction between precursor molecules and surface materials. Therefore, the chemical conditions of the BP surface will have an impact on the nucleation or growth of oxide layers.

Zhou et al. conducted in-situ interface studies on BP, and found that the interface chemistry and phosphorus oxide species can affect the nucleation/growth of Al_3 on the BP surface [10]. The results show that surface oxidation states play a key role in the growth of ALD. Aluminum hydroxide oxides have advantages in thickness, conformal coating and scalability, but the interfacial chemistry needs to be carefully controlled to avoid unwanted BP modification.

5.2. Polymer-Based Encapsulation

Polymer encapsulation is another method to improve BP environmental stability [14-16]. Polymers like PMMA, hydrophobic polymers can reduce BP's direct exposure to atmospheric oxygen and water.

Jia et al. used PMMA passivation to study plasma-treated BP, and the passivated BP device could retain electrical characteristics and have better environmental stability after several weeks [14]. This shows that polymers can play a useful role in the protection of BP electronic devices.

Other studies have explored the encapsulation of hydrophobic polymer to improve the stability or reliability of the BP transistors. Polymer-based protection is compared with traditional aluminum-O_3 coating, which shows that it can protect BP under environmental or electrical stress [15].

Polymer-based BP hybrid materials have been developed through in-situ radical polymerization. This method can stabilize the nanoflakes of BP and improve the resistance to environmental degradation [16].

Polymer encapsulation has limitations. Process residues, trapped pollutants, interface quality and thermal stability are important [15,16]. Polymers have physical or chemical changes at high temperatures or long-term environmental exposure.

Polymer coatings are attractive, because they are relatively simple to process and have good passivation, but the long-term stability of the interface and the quality of interface need to be considered.

5.3. Advantages of h-BN Compared with Conventional Protective Layers

The two-dimensional structure of H-BN can protect BP without thick coating, and its chemical stability can resist atmospheric degradation [11-13].

The key advantage is that van der Waals interfaces with BP, which reduces the need for strong chemical bonds, and can also reduce the chemical modification of the surface of BP [11,12]. Therefore, h-BN provides a relatively clean interface and is also an environmental obstacle.

The three methods have different advantages. The ALD oxides can control thickness, conformal coverage and are suitable for scalable manufacturing, but their deposition requires surface chemical reactions [8,10]. Polymer coating is easy to process and has good passivation ability, but interface contamination or thermal stability may limit long-term performance [14-16]. H-BN has a flat,

chemically stable and electrically insulated interface, and large-area manufacturing and transfer are still relatively challenging [11-13].

Therefore, h-BN is not a universal replacement for traditional encapsulation methods. Its main advantage lies in balancing environmental protection and the properties of two-dimensional semiconductors.

6. Limitations and Future Perspectives

H-BN encapsulation has advantages, but there are challenges before large-scale BP technology is widely applied.

The first challenge lies in large-area manufacturing. High-quality H-BN flakes are obtained by mechanical exfoliation. However, the size, thickness and uniformity of expfoliated flakes will be difficult to precisely control. Laboratory devices can benefit from h-B encapsulation, and large-scale manufacturing requires more scalable methods.

The second challenge lies in the transfer process. When h-BN is transferred to BP, bubbles, polymers, and other contaminants will enter the interface. These defects will reduce the quality of van der Waals interfaces, and also cause local electronic properties to change.

Edge protection is an important issue. Even if the top and bottom surface of BP are covered, the exposed edges may provide a path for oxygen or moisture to reach active layers. Future encapsulation designs need to consider surface protection and complete protection of device edges.

Integrating with traditional semiconductor manufacturing is an obstacle. Practical devices need to perform reproducible processing, be accurate, have low contamination, and be compatible with existing manufacturing technologies. Deterministic transfers, wafer h-BN growth growth and automated stacking methods can play an important role in the development of BP devices.

Interface engineering is a key research direction. Control the thickness of h-BN, cleanliness of the interface, stacking configuration and contact geometry, so as to optimize the balance of environmental protection and the performance of electronic devices.

The hybrid encapsulation strategy may provide a promising solution. For example, combining H-BN with oxide/polymer layers may combine the clean interface and the advantages of large-area processing of traditional protective films. This method may be able to overcome the limitations of single encapsulation materials.

Finally, scalable and repeatable encapsulation technology is very important if BP is to shift from laboratory demonstrations to practical two-dimensional semiconductor application.

7. Conclusion

Black phosphorus has a tunable bandgap (bandgap), high carrier mobility (carrier mobility), strong in-plane anisotropy (i.e., excellent infrared optical response), and is a promising two-dimensional semiconductor suitable for future electronic and optical applications. However, poor atmospheric stability is the main obstacle to practical application.

When exposed to oxygen, moisture and light, the degradation of BP will lead to oxidation, structural defects and changes in electronic properties. Oxygen plays an important role in degradation, while light will accelerate oxidation through photo-induced processes. These changes will increase carrier scattering, and also reduce the performance or reliability of BP-FETs and optical devices.

H-BN encapsulation is a promising way to solve this problem. In the structure of h-B/BP/h-BN, the h-B layer acts as a physical barrier, reducing BP's exposure to oxygen and moisture. H-BN interfaces with BP, reducing strong chemical bonds and reducing potential chemical modification on the BP surface.

H-BN has characteristics such as chemical stability (chemical stability), atomic flatness (atomic flat), electrical insulation (electric insulation), and clean van der Waal interface (vib). ALD is attractive because of precise thickness control (thin control) and scalability (scalability), while polymer coatings are relatively simple and effective passivation. However, when preserving the intrinsic properties of two-dimensional semiconductors is a key priority.

However, the encapsulation of h-BN is not completely free of disturbances. Dielectric detection, interface charge, strain, transfer residue, bubbles, defects and edge leakage will still have an impact on BP device properties and reliability. So h-B is a low-density encapsulation strategy, which can achieve environmental protection while reducing the changes in BP intrinsic properties.

Overall, the encapsulation of h-BN is an important method for improving black phosphorus atmospheric stability. It combines environmental protection with a clean two-dimensional interfaces, which is very promising for stable BP electronic/optical devices. However, challenges such as large-area fabrication, transfer-induced contamination, edge protection and scalable device integration still need to be solved. The development of interfaces, deterministic transfers, wafer-scale h-B production, hybrid encapsulation strategies, etc., may make BP devices more reliable and scalable. If these challenges are effectively addressed, the protected black phosphorus protected by h-BN may become a key platform for future two-dimensional semiconductor technology.

References

[1] Xia F, Wang H, Jia Y. Rediscovering black phosphorus as an anisotropic layered material for optoelectronics and electronics. Nature Communications, 2014, 5: 4458.

[2] Li L, Yu Y, Ye G, et al. Black phosphorus field-effect transistors. Nature Nanotechnology, 2014, 9(5): 372-377.

[3] Liu H, Neal A T, Zhu Z, et al. Phosphorene: An unexplored 2D semiconductor with a high hole mobility. ACS Nano, 2014, 8(4): 4033-4041.

[4] Ossila. Black phosphorus structure. https://www.ossila.com/pages/black-phosphorus-structure.

[5] Abate Y, Akinwande D, Gamage S, et al. Recent progress on stability and passivation of black phosphorus. Advanced Materials, 2018, 30(29): 1704749.

[6] Huang Y, Qiao J, He K, et al. Interaction of black phosphorus with oxygen and water. Chemistry of Materials, 2016, 28(22): 8330-8339.

[7] Favron A, Gaufrès E, Fossard F, et al. Photooxidation and quantum confinement effects in exfoliated black phosphorus. Nature Materials, 2015, 14: 826-832.

[8] Wood J D, Wells S A, Jariwala D, et al. Effective passivation of exfoliated black phosphorus transistors against ambient degradation. Nano Letters, 2014, 14(12): 6964-6970.

[9] Illarionov Y, Waltl M, Rzepa G, et al. Long-term stability and reliability of black phosphorus field-effect transistors. ACS Nano, 2016, 10(10): 9543-9549.

[10] Avsar A, Vera-Marun I J, Tan J Y, et al. Air-stable transport in graphene-contacted, fully encapsulated ultrathin black phosphorus-based field-effect transistors. ACS Nano, 2015, 9(4): 4138-4145.

[11] Arora H, Fekri Z, Vekariya Y N, et al. Fully encapsulated and stable black phosphorus field-effect transistors. Advanced Materials Technologies, 2023, 8(2): 2200546.

[12] Birowska M, Urban J, Baranowski M, et al. The impact of hexagonal boron nitride encapsulation on the structural and vibrational properties of few layer black phosphorus. Nanotechnology, 2019, 30(19): 195201.

[13] Zhu H, McDonnell S, Qin X, et al. Al_2O_3 on black phosphorus by atomic layer deposition: An in situ interface study. ACS Applied Materials & Interfaces, 2015, 7(23): 13038-13043.

[14] Jia J, Jang S K, Lai S, et al. Plasma-treated thickness-controlled two-dimensional black phosphorus and its electronic transport properties. ACS Nano, 2015, 9(9): 8729-8736.

[15] Li X, Wu J, Ye Y, et al. Performance and reliability improvement under high current densities in black phosphorus transistors by interface engineering. ACS Applied Materials & Interfaces, 2019, 11(1): 1587-1594.

[16] Passaglia E, Cicogna F, Costantino F, et al. Polymer-based black phosphorus (bP) hybrid materials by in situ radical polymerization: An effective tool to exfoliate bP and stabilize bP nanoflakes. Chemistry of Materials, 2018, 30(6): 2036-2048.