Introduction of 2D Materials Heterostructures' Properties

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Abstract: Since the successful fabrication and characterization of graphene, it has demonstrated many unprecedented exceptional properties, garnering extensive attention and research interest. Simultaneously, studies on graphene have propelled the development of research into other two-dimensional (2D) materials. Research in this field has achieved significant breakthroughs and rapid progress, establishing itself as a prominent focus in condensed matter physics and materials science. Initially, studies on 2D materials primarily concentrated on single-layer 2D materials. Later, researchers discovered that stacking two or more different 2D materials could also result in the formation of novel 2D materials, collectively referred to as 2D material heterostructures. 2D materials science due to their unique nanoscale properties. These heterostructures demonstrate remarkable optical and electronic characteristics, making them ideal candidates for the development of atomically thin devices. This review summarizes recent advancements in 2D material heterostructure research and explores potential future directions and developments in this rapidly evolving field.

Keywords: Graphene, 2D Materials, 2D Material Heterostructures

1. Introduction

Graphene is a 2D crystalline arrangement of carbon atoms in a honeycomb lattice, serves as the foundational structural unit for all graphitic materials, encompassing 0D fullerenes, 1D carbon nanotubes, and 3D graphite (Figure 1). Graphene exhibits exceptional properties unmatched by other graphitic forms, including a Young's modulus of 1TPa, intrinsic strength of 130GPa, and thermal conductivity exceeding 3,000W mK⁻¹. It is completely impermeable to any gases and supports extremely high current densities, surpassing copper by six orders of magnitude[1].

Graphene's charge carriers can be modulated between electrons and holes at carrier concentrations up to 10^{13} cm⁻². Under ambient conditions, graphene exhibits a carrier mobility exceeding 15,000 cm²V⁻¹s⁻¹, with a weak temperature dependence indicative of impurity-limited scattering, suggesting potential mobility as high as 100,000 cm²V⁻¹s⁻¹. Unlike undoped bulk semiconductors, graphene retains high mobility at carrier concentrations exceeding 10^{12} cm⁻² in both electrically and chemically doped devices[2].

These extraordinary properties position graphene as a promising candidate for various advanced technologies, including printable and flexible electronics, flexible photovoltaics, and supercapacitors[1]. Additionally, graphene has demonstrated potential in spintronic devices,

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superconducting field-effect transistors, and hydrogen storage applications, underscoring its versatility and suitability for future technological innovations[2].



Figure 1: Graphene as the Fundamental Structure of All Graphitic Forms. Graphene, a twodimensional material, serves as the foundational building block for carbon structures of various dimensionalities. It can be enclosed into 0D fullerenes (buckyballs), rolled into 1D carbon nanotubes, or stacked into 3D graphite[2].

2. Fabrication

In the preparation of graphene, one approach is to extract graphene from bulk graphite via mechanical exfoliation (Figure 2). This technique has successfully produced high-quality graphene microcrystals with sizes up to 100 μ m[2]. Under an optical microscope, these graphene samples can be readily observed and differentiated between monolayer and bilayer graphene, with bilayer graphene formed by the folding of a single graphene layer (Figure 3).

The graphene samples produced through this method are typically deposited on a silicon substrate with a SiO₂ surface layer of a specific thickness, which is crucial for making the graphene visible under an optical microscope. A small variation in the SiO₂ thickness (e.g., changing from 300 nm to 315 nm) can render the graphene completely invisible[2]. When observed under an atomic force microscope (AFM), thicknesses of approximately 9 Å and 13 Å can be clearly observed, with the 13 Å region also resulting from folded monolayer graphene (Figure 4). Scanning electron microscope (SEM) imaging reveals that most graphene crystal edges exhibit zigzag and armchair configurations, as denoted by the blue and red lines in Figure 5.



Figure 2: Mechanical exfoliation of graphene from bulk graphite[1].



Figure 3: Optical microscopy image of graphene layers on a Si substrate with a 300 nm thick SiO₂ layer [3].



Figure 4: Graphene visualized using atomic force microscopy. (Copyright National Academy of Sciences, USA.)



Figure 5: Scanning electron micrograph of a relatively large graphene crystal[2].

Large-area graphene films can be prepared by chemical vapour deposition (CVD) on copper films. At smaller scale, graphene films produced by CVD exhibit electronic transport properties comparable to those of exfoliated graphene on SiO₂ and hexagonal boron nitride (h-BN) substrates. Despite the presence of some defects, these films remain suitable for applications in transparent conductive coatings[1]. However, widespread adoption of CVD technology remains limited, primarily due to high production costs and challenges in precisely controlling graphene growth during synthesis. The high costs are largely attributed to substantial energy requirements and the necessity of removing the metal layer post-deposition. Advances in graphene transfer methods are anticipated to enhance cost-effectiveness. Critical challenges for future research include achieving graphene growth on metal films only tens of nanometers thick and gaining control over parameters such as grain size, ripple formation, doping levels, crystallographic orientation, and the number of growth layers[1].

The promising properties of graphene have sparked interest in other two-dimensional (2D) atomic crystals. Like graphene, these materials can be synthesized through mechanical exfoliation or chemical vapor deposition (CVD). Beyond these methods, distinct types of 2D atomic crystals can be stacked to create multilayer "sandwich" structures, as illustrated in Figure 6. This approach enables the formation of new 2D materials, collectively termed 2D material heterostructures. By layering different materials, these heterostructures can exhibit physical properties distinct from those of the individual layers.

3. **Properties**

The family of 2D atomic crystals is broad, featuring a variety of unique characteristics, which means that heterostructures composed of different 2D materials hold substantial potential for diverse functionalities. Commonly utilized 2D atomic crystals for creating heterostructures include graphene (GE), boron nitride (BN), and molybdenum disulfide (MoS₂). In Figure 6, the second layer from the bottom —the thickest layer in the image— is MoS₂. This layer interacts with the graphene layer (blue in the image), generating a built-in electric field that separates electron-hole pairs and thus produces a photocurrent. Several layers of boron nitride (shown in yellow and purple) separate the two graphene layers, providing insulation and protecting the graphene.[1].



Figure 6: 3D demonstration of optically active 2D heterostructure[1].

The quantum Hall effect is a fundamental phenomenon often discussed in the context of 2D materials. For instance, in graphene (Figure 7), the Hall conductivity σ_{xy} (represented by the red line in the figure) displays a series of uniform, equidistant steps. At the neutrality point —also referred to as the Dirac point—the resistance (indicated by the blue line) reaches its maximum value, marking the transition of charge carriers from electrons to holes[2].

In Figure 8, the inset in the upper right corner shows an optical microscope image of a graphene Hall bar. The graph illustrates the variation of the Hall bar's resistance as a function of the gate voltage.

Notably, at the Dirac point, the resistance attains its peak value, approximately $4 \text{ k}\Omega$. The inset in the upper left corner provides a depiction of graphene's low-energy dispersion[4].



Figure 7: Quantum Hall effect in graphene[2].



Figure 8: Resistance of graphene measured at 1.7K at different gate voltages[4].

Under certain conditions, 2D materials can exhibit ferroelectric properties, becoming ferroelectrics by generating spontaneous polarization that can be reversed by an external electric field. Figure 9 shows the structure of a 2D ferroelectric semimetal, fabricated using the dry-transfer technique with quasi-twisted bilayer graphene (qTBG) [5-6]. In this configuration, the graphene layers in qTBG are separated by a monolayer hexagonal boron nitride (mhBN) and encapsulated by two relatively thicker hBN flakes. This structure is both electron transparent and shielded from external environmental influences. Furthermore, top and bottom gate electrodes allow independent control over the carrier density in the two graphene layers[6].

Top gate	
hBN	
-O-MLG-O-O	
0−hBN -0-0	
-0-MLG-0-0	5
hBN	
SiO ₂	
Back gate	

Figure 9: Ferroelectric semimetal made of double-gated double-layer graphene separated by an atomically thin crystal of hexagonal boron nitride[6].

Figure 10 shows the resistivity of the sample structure as a function of back-gate voltage (V_{bg}) and top gate voltage (V_{tg}) , with measurements taken at $V_{tg} = 0$ V, $V_{bg} = 0$ V, and a temperature of 2.1 K. In the resistivity versus V_{bg} plot, when the gate voltage sweep direction is reversed, the charge neutrality points (CNPs) corresponding to maximum resistivity values, are separated by more than 10 V, indicating a stable hysteresis effect. This hysteresis effect is consistently observed across multiple voltage sweep cycles, with no evidence of degradation. A similar hysteresis effect is observed during the top gate voltage sweep as well [6].



Figure 10: The device's resistivity measured as a function of V_{bg} and V_{tg} at 2.1K for $V_{tg}=0$ V and $V_{bg}=0$ V, respectively[6].

Unconventional superconductivity is a notable feature of certain 2D materials. In twisted bilayer graphene (TBG), when the twist angle between the two graphene layers is approximately 1.1° , the electronic band structure forms flat bands near the Fermi energy, leading to a correlated insulating state at half-filling. By moving away from this correlated insulating state through electrostatic doping, unconventional superconductivity emerges within the TBG superlattice [7]. This superlattice has a period of about 13 nm, as shown in the lower right inset of Figure 11. The two monolayer graphene sheets, G1 and G2, are derived from a single exfoliated graphene flake, enabling precise control of the twist angle to within an accuracy range of $0.1^{\circ}-0.2^{\circ}$ [7].

Figure 12 illustrates the temperature-dependent longitudinal resistance for two TBG devices, M1 and M2, with twist angles of 1.16° and 1.05°, respectively. The inset presents an optical microscopy image of device M1, showing the Hall bar structure fabricated from the encapsulated TBG stack, with the Hall bar in dark brown, electrical contacts in gold, the back gate in light green, and the SiO₂/Si substrate in dark gray[7].



Figure 11: Schematic of a typical TBG device and the four-probe (V_{xx} , V_g , I and the bias voltage V_{bias}) measurement scheme[7].

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Figure 12: Four-probe resistance $R_{xx} = V_{xx}/I$ (V_{xx} and I are defined in figure 11) measured in two devices M1 and M2[7].

Unconventional superconductivity has also been observed in twisted trilayer graphene (TTG). In the atomic reconstruction regions of TTG, symmetry-breaking electronic transitions and dopingdependent band structure deformations, similar to those found in TBG, have been observed[8]. Figure 13 depicts the setup for observing TTG via scanning tunneling microscopy (STM). In this setup, TTG is placed on a hBN substrate, with doping controlled by a graphite back gate.

Figure 14 shows the topography of TTG with an alternating twist angle of 1.5°Theoretically, three graphene layers could form two independent moiré patterns; however, the observed moiré pattern consistently appears as a single triangular lattice without additional patterns. This observation suggests that in the studied TTG, the first and third graphene layers are aligned, while the middle layer is twisted by 1.5° [8].



Figure 13: Schematic of the STM experiment[8].



Figure 14: A 26 nm by 26 nm topographic image showing moiré lattice structure with a moiré periodicity of approximately 9 nm. The scale bar represents 10 nm. Inset: the atomic-scale hexagonal lattice of carbon atoms , with a scale bar of 0.5 nm[8].

4. Conclusion

This paper examines the optical and electrical properties of graphene and other two-dimensional (2D) material heterostructures, with a particular focus on the quantum Hall effect, ferroelectric properties, and unconventional superconductivity. Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has emerged as a transformative material due to its exceptional electronic, thermal, and mechanical properties. Its high electron mobility, thermal conductivity, and transparency have paved the way for numerous applications, from transparent conductive films to advanced transistors.

In summary, graphene and other 2D materials hold immense promise for the future of electronics, photonics, and quantum technologies. Continued research into the synthesis, stacking, and manipulation of 2D materials will be crucial for realizing their full potential in commercial applications, particularly in next-generation transistors, flexible electronics, and high-performance optoelectronic devices. By addressing the challenges in material synthesis and interface control, the field of 2D materials is poised to make significant contributions to the advancement of modern technology and fundamental physics. In summary, graphene exhibits remarkable thermal conductivity, ferroelectric, and superconducting properties, underscoring its significant potential for research and applications in 2D material heterostructures and advanced electronic devices.

References

- [1] K. S. Novoselov, V. I. Fal'Ko, L. Colombo, P. R. Gellert, M. G. Schwab, and K. Kim, 'A roadmap for graphene', Oct. 11, 2012. doi: 10.1038/nature11458.
- [2] A. K. Geim and K. S. Novoselov, 'The rise of graphene'. [Online]. Available: www.nature.com/naturematerials
- [3] V. V. Strelchuk, A. S. Nikolenko, V. O. Gubanov, M. M. Biliy, and L. A. Bulavin, 'Dispersion of electron-phonon resonances in one-layer graphene and its demonstration in micro-raman scattering', J Nanosci Nanotechnol, vol. 12, no. 11, pp. 8671–8675, Nov. 2012, doi: 10.1166/jnn.2012.6815.
- [4] Y. Zhang, Y. W. Tan, H. L. Stormer, and P. Kim, 'Experimental observation of the quantum Hall effect and Berry's phase in graphene', Nature, vol. 438, no. 7065, pp. 201–204, Nov. 2005, doi: 10.1038/nature04235.
- [5] A. V. Kretinin et al., 'Electronic properties of graphene encapsulated with different two-dimensional atomic crystals', Nano Lett, vol. 14, no. 6, pp. 3270–3276, Jun. 2014, doi: 10.1021/nl5006542.
- [6] W. Yibo, 'Ferroelectricity in hBN intercalated double-layer graphene', 2022.
- [7] Y. Cao et al., 'Unconventional superconductivity in magic-angle graphene superlattices', Nature, vol. 556, no. 7699, pp. 43–50, Apr. 2018, doi: 10.1038/nature26160.
- [8] H. Kim et al., 'Evidence for unconventional superconductivity in twisted trilayer graphene', Nature, vol. 606, no. 7914, pp. 494–500, Jun. 2022, doi: 10.1038/s41586-022-04715-z.