【系所領航】薛宏中許誌恩與成大臺大國輻中心合作 首創二維鐵電材料登頂國際期刊

學習新視界

【記者陳宇暄淡水校園報導】物理學系教授暨研發處研發長薛宏中、理學院應用博三許誌恩，與成功大學、國家同步輻射研究中心、臺灣大學凝態科學研究中心組成研發團隊，共同發表「Epitaxial Ferroelectric Hexagonal Boron Nitride Grown on Graphene（在石墨烯上外延生長的鐵電性六方氮化硼）」，4月刊登於國際頂尖期刊《Advanced Materials》（先進材料），影響因子為27.4，5年影響因子更高達30.2。

該團隊研究首度在石墨烯上成功堆疊出「具有鐵電性的超薄六方氮化硼（h–BN）薄膜」，並證實其能穩定地切換電極極性，研究成果顯示，h–BN/石墨烯異質界面的莫爾（Moire）超晶格導致自發極化，而層間滑移可實現可逆極化切換，以此證明其鐵電特性。「鐵電性」如同材料內部具有一個可自由切換的電極性開關，能精確控制電流流向，尤其適合用於記憶體、感測器及低功耗運算裝置。

薛宏中表示，成大教授吳忠霖團隊採用「電漿輔助分子束磊晶技術（MBE）」，在碳化矽晶片上先成長高品質單晶石墨烯，再於其上逐層精準堆疊h–BN，藉由在介面自然形成的摩爾紋（Moir Pattern），誘導出具非對稱且可透過電場切換堆疊的極化結構。國輻中心研究員鄭澄懋表示，團隊運用國輻中心的台灣光源（Taiwan Light Source, TLS），進行角解析光電子能譜（ARPES）量測，清楚觀測到不同層數h–BN，與石墨烯異質結構中的能帶變化。薛宏中與許誌恩運用第一原理基態（密度泛函理論DFT）與激發態（GW多體微擾修正），計算驗證其層間極化機制，及非對稱鐵電堆疊結構的存在與特徵。

這項成果為二維鐵電材料的異質外延，與可調控電子元件應用提供了新契機，未來可透過堆疊式異質結構晶片的設計，推動臺灣半導體及光電產業的重大技術革新。薛宏中表示，透過此次與成大、臺大實驗團隊及國輻中心合作，展現本校物理系在理論與實驗研究的整合能力，並提供學生參與國際尖端研究的機會。


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Epitaxial Ferroelectric Hexagonal Boron Nitride Grown on Graphene

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Ferroelectricity realized in van der Waals (vdW) materials with non-centrosymmetric stacking configurations holds promise for future 2D devices with nonvolatile and reconfigurable functionalities. However, the epitaxial growth of ferroelectric vdW materials often struggles to achieve an energetically unfavorable stacking configuration that enables electric polarization. This challenge is particularly evident when performing heteroepitaxy on another vdW substrate to create versatile and scalable ferroelectric building blocks designed for large-area, atomic-scale thicknesses. Here, epitaxial hexagonal boron nitride (h-BN) multilayer films are successfully grew on single-crystal graphene synthesized on a miscut SiC (0001) substrate. Theoretical calculations illustrate that the moiré-patterned h-BN/graphene hetero-interface intrinsically exhibits polarization, leading to a polarized AB stacking in multilayer h-BN films to minimize the total formation energy, which is validated experimentally by the layer-dependent band dispersions. The as-grown multilayer h-BN layers demonstrated robust, homogeneous ferroelectricity with switchable out-of-plane polarization via interlayer sliding. This study establishes an effective route for stacking-controlled heteroepitaxy, enabling the large-scale integration of vdW materials with ferroelectricity and versatile functionalities, offering a promising platform for next-generation 2D ferroelectric devices.

1. Introduction

The realization of ferroelectricity at atomic-scale thickness, i.e., 2D ferroelectrics, has shown great promise for driving device innovation in the post-Moore era, where efficient energy storage and dense digital information retrieval at reduced dimensions are critical.[1–15] In naturally grown van der Waals (vdW) diatomic crystals, such as hexagonal boron nitride (h-BN) and transition-metal dichalcogenides (TMDs), electric polarization arising from layer stacking is typically absent due to the lower formation energy of these centrosymmetric crystals compared to non-centrosymmetric stacking configurations. Through manual micromechanical exfoliation and restacking processes to break the crystallographic inversion symmetry, out-of-plane electric polarization was generated in twisted h-BN stacked sheets by forcing the rotational and translational in-plane shifts between two non-polar h-BN layers.[1–4] This discovery of ferroelectricity in twisted

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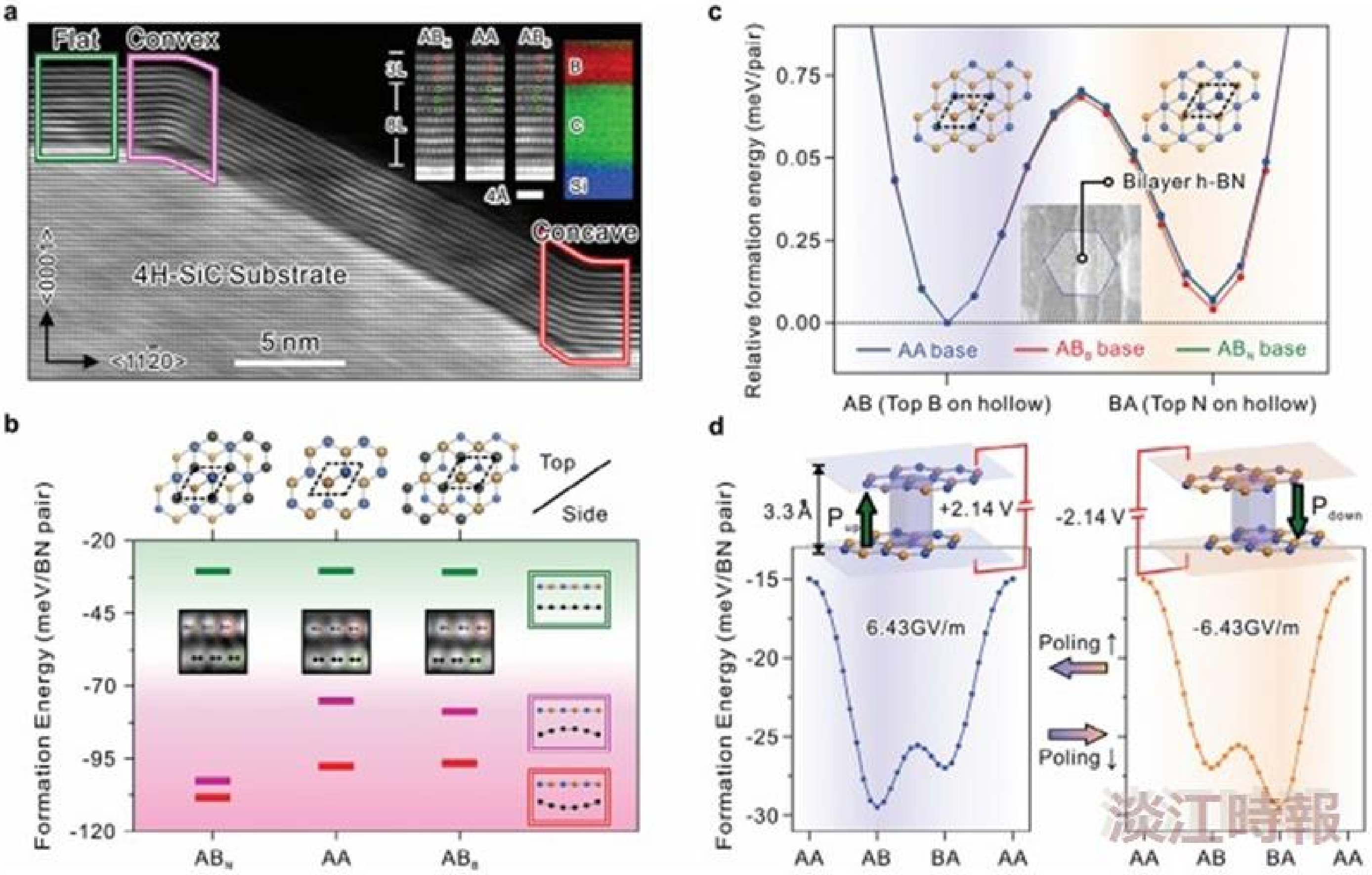
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Flat
Convex
Concave
4H-SiC Substrate
5 nm
<0001>
<11-20>
AA
4Å
B
C
Si
b
Top
Side
Formation Energy (meV/BN pair)
-20
-45
-70
-95
-120
AB
AA
AB
c
Relative formation energy (meV/pair)
0.75
0.05
0.25
0.00
Bilayer h-BN
AA base
AB base
AB base
AB (Top B on hollow)
BA (Top N on hollow)
d
3.3Å
+2.14 V
-2.14 V
Formation Energy (meV/BN pair)
-15
-20
-25
-30
6.43GV/m
-6.43GV/m
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