Dislocations in Bilayer Transition Metal Dichalcogenides

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Van der Waals epitaxy allows to release the lattice matching condition dramatically with weak interface interaction. Here, we demonstrate that stacking boundaries in tungsten disulfide (WS_2) film in the WS_2 and graphene heterostructure, which means that van der Waals epitaxy has non-negligible interaction at interface. WS_2 films including stacking boundaries are synthesized directly on graphene substrate, which includes large grain size and wrinkles. Stacking boundaries[1,2], one of topological defects, are facilitated by Shockley partial dislocations in bilayer two-dimensional (2D) materials, which cannot escape. Stacking boundaries have been researched actively, especially in the case of bilayer graphene, because it can be applicable to various applications, such as valleytronics[3]. Transition metal dichalcogenides (TMDs), which are representative bi-elemental 2D material, have various stacking structure, according to the orientation and translation. However, there has been no any experimental results, representing AB/AC stacking boundary TMDs, due to the finite flake size and random orientation of TMDs domains on silica substrate, which results in preference of grain boundary.

In this paper, AB/AC stacking boundary and partial dislocations in TMDs were analysed using scanning transmission electron microscopy (STEM) and dark-field (DF) TEM methods. Using the scanning electron microscopy (SEM) image with high field-of-view, multilayer WS_2 and different stacking regions are synthesized along the graphene wrinkles, deducing the relations between wrinkle in substrate and topological defects in film. Wrinkles in graphene are known as nucleation site with high chemical reactivity[4]. In addition, we suggest wrinkles act as vertical barrier with vertical height, which induce additional stress to the epitaxially grown film, apart from difference of thermal expansion coefficient between substrate and film. AB/AC stacking boundaries in bilayer WS_2 are strain-mediated nanometer-wide channels, without any charge redistribution. Atomic force microscopy (AFM) represents stacking boundaries buckle with around 1 nm vertical height for reducing in-plane strain via the out-of-plane distortion[1]. Our simulation results demonstrate that buckled structure is more favourable energetically, which correspond to experimental results. In addition, we performed band gap calculations according to in-plane strain. It results in reduced band gap for strained flat stacking boundary, on the other hands, restored band gap for buckled stacking boundary with relaxed strain. Furthermore, for increased stacking boundary width, stacking boundaries behave as monolayer TMDs due to the increased interlayer distance via buckling. Our results provide a new understanding of graphene morphology mediated novel stacking boundaries and corresponding properties in bilayer WS_2 for the first time, which might be applied to various applications.

References

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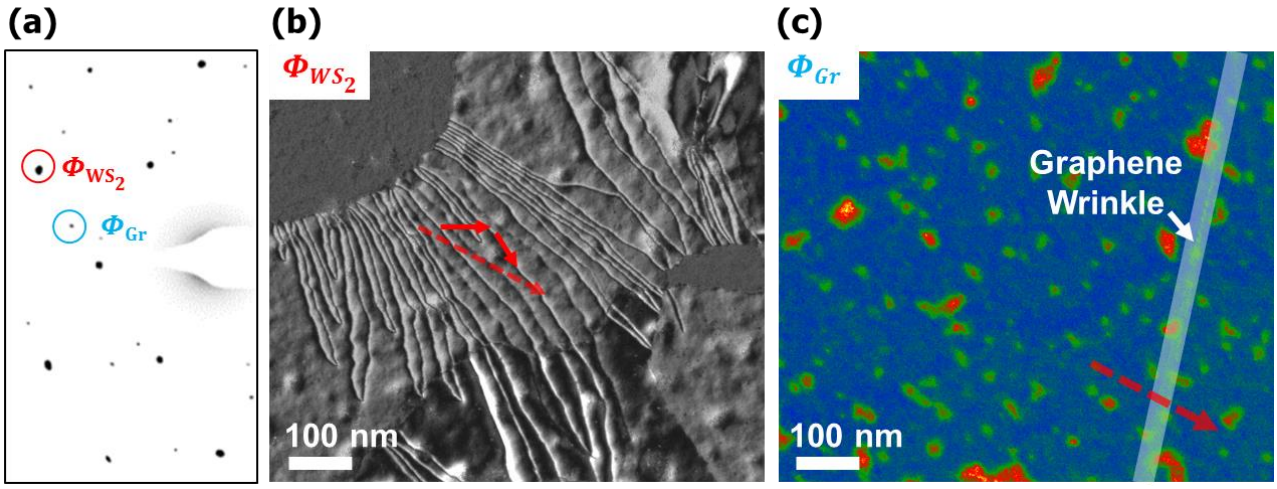

Figure 1. (a) Diffraction pattern of WS_2 and graphene heterostructure. (b) DF-TEM images representing AB/AC stacking and stacking boundaries induced by partial dislocations. The dislocation is related with graphene wrinkle as shown in (c). Red solid-arrow and dash-arrow means burgers vectors of partial dislocations and direction of basal plane dislocations.