Resonant Tunneling Detection of Atomic Reconstruction in Twisted Bilayer WSe_2

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A moiré lattice in a twisted-bilayer (tBL) transition metal dichalcogenide exhibits a complex atomic reconstruction when its twist angle is less than a few degrees [1]. In this study, we perform resonant-tunneling transport measurements and transmission electron microscopy (TEM) observations for tBL-WSe_2 samples with various twist angles, and reveal the correlation between atomic reconstruction and the subband energy at the valence band (VB) Γ point.

A schematic of tunneling devices is presented in Fig. 1(a). Under an application of gate voltages and interlayer bias V_{int}, a hole tunnel current I flows from 3L-WSe_2 into tBL-WSe_2 through the *h*-BN barrier. Resonant tunneling occurs when the energy of the VB top at the Γ-point of 3L-WSe_2 coincides with the energies of the VB Γ-point band of d-WSe_2, with energy and momentum conservation [2,3]. Consequently, a peak current with negative differential resistance emerges in the I-V_{int} curve, allowing us to probe the VB Γ-point energies of tBL-WSe_2. Fig. 1(b) shows the results of tunneling into tBL-WSe_2 under different twist angles θ_{BL}. The observed two peaks, indicated by red and blue marks, correspond to resonant tunneling into VB-Γ-point states of tBL-WSe_2. These V_{int} positions are plotted against θ_{BL} in Fig. 1(c). The results indicate a significant change in the VB-Γ point band at small twist angle region such as $\theta_{\mathrm{BL}} = 0°$, 2°, and 4°, as illustrated in Fig. 1(d). In this twist angle region, we observed an atomic-reconstructed moiré lattice in tBL-WSe_2 by using TEM (Fig. 1(e)). Thus, the band alternations are attributed to the atomic reconstruction in tBL-WSe_2. Our calculations indicate that the VB-Γ-point band of BL-WSe_2 is significantly affected by the interlayer distance. Therefore, we consider that the atomic reconstruction influences the interlayer distance, consequently modifying the VB-Γ-point energies. Our findings highlight the energy changes associated with lattice alterations due to the atomic reconstruction in tBL-WSe_2, providing a different viewpoint from the well-explored energy modulations by the moiré potentials.

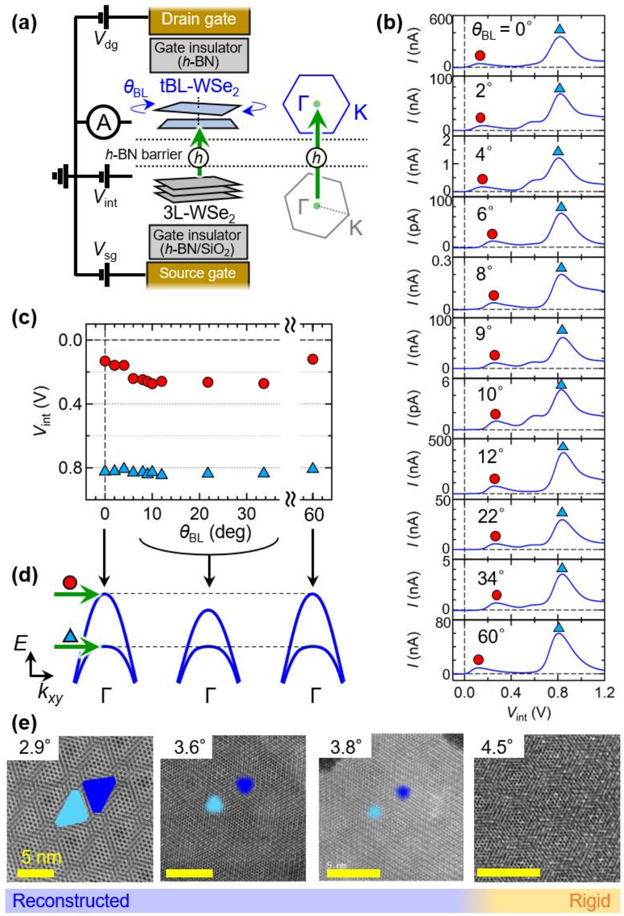

Fig. 1 (a) Schematics of the tunneling device and momentum-conserved resonant tunneling. (b) Current-voltage characteristics from all the devices. (c) Peak V_{int} positions plotted against θ_{BL}. (d) Schematics of twist angle dependence of the VB-Γ-point band of tBL-WSe_2. (e) TEM images of tBL-WSe_2. Blue (light blue) marks indicate the atomic-reconstructed features. All scale bars are 5 nm.

References

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