P:26 Impact of layer rotational misalignment on the transport properties of van der Waals tunnel field effect transistors

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2D materials are a promising option for the realization of ultra-low-power tunnel field effect transistors (TFETs) thanks to their thinness, the absence of dangling bonds and the large band structure variety [1]. In this work, we study the impact of layer misorientation on the transport properties of a vertical TFET based on a MoS_2/WTe_2 van der Waals (vdW) heterojunction [2]. To this aim, we use an effective mass Hamiltonian model and the non-equilibrium Green's function approach self-consistently coupled with the 3D Poisson equation for an accurate description of the system electrostatics. The effect of electron-phonon interaction is included within the self-consistent Born approximation. We consider both acoustic phonons within the elastic approximation and dispersionless optical phonons with parameters taken from [3].

The simulated vdW-TFET is shown in Fig. 1(a) and consists in a WTe_2 bottom layer acting as source and a MoS_2 top layer acting as drain. When the MoS_2 and the WTe_2 monolayers are stacked with a relative rotation angle θ, the hexagonal Brillouin zones of the two original layers are also rotated by θ around the Γ point, as shown in Fig. 1(b).

Hence, the MoS_2 conduction bands with valleys at the K and K' points are shifted from the corresponding WTe2 valence bands, thus resulting in indirect band gaps between the two layers.

Fig. 2(e) shows the transfer characteristic IDS-VTG of the device for different rotation angles θ = 0, 10.5° and 21°. As can be seen, the rotational misalignment determines a significant current decrease. As schematized in Fig. 2(a-d), this is due to the interlayer tunneling reduction induced by the valley shift, which implies that a larger momentum change is needed by electrons to pass from one band to the other one. The impact on the subthreshold swing (SS) is quite modest, whereas the on-state current depends considerably on the rotation angle.

To analyze this behavior, Fig. 3 shows the interlayer tunneling current density for the vdW-TFET in the on-state with θ = 10.5° and θ = 21°. As shown in Fig. 3(a), for relatively small rotation angles, the tunneling occurs inside the overlap region. On the contrary, for larger angles the tunneling is localized at the edges of the overlap region, see Fig. 3(b), while it is very weak in the central area due to the fact that phonons alone are not able to scatter the electrons over a large Δk.

Conversely, the sharp edges of the overlap region are source of short-range scattering, and thus allow the electrons to change their momentum and to tunnel between the shifted valleys.

Since at room temperature the interlayer tunneling can be assisted also by phonons, in Figs. 4(a,b), we consider the most unfavorable configuration (θ = 21°) for the vdW-TFET and artificially tune the deformation potential for acoustic (D_{ac}) and optical phonons (D_{op}). The increase of the phonon scattering strength results in a substantial on-current enhancement. As illustrated in Fig. 2(d), the electron tunneling can be triggered by two different mechanisms: one is the change of the momentum and the other is the optical phonon absorption, which promotes electrons to higher energy levels. Figs. 4(a,b) indicate that an increase of D_{ac} and D_{op} results in similar on-state currents, which suggests that the increase of IDS is more likely due to the momentum scattering.

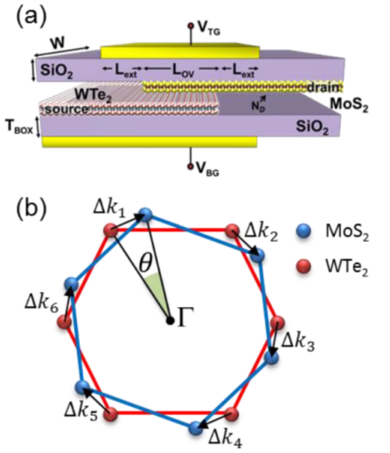

Figure 1. (a) Simulated van der Waals TFET. Tunnelling, driven by the top gate potential V_{TG}, occurs in the overlap region. (b) Brillouin zones (red and blue hexagons) of the two misoriented monolayers. The indirect gaps are indicated by the six vectors Δk_i.

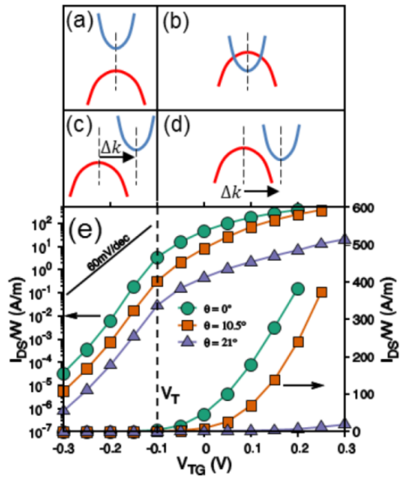

Figure 2. Schematics of the alignment of the MoS_2 conduction and WTe_2 valence bands (a,b) without and (c,d) with rotational misalignment. With the rotation, the band gap becomes indirect with a shift vector Δk. Panels (a,c) correspond to the subthreshold $V_{TG}<V_T$, and panels (b,d) correspond to $V_{TG}>V_T$. (e) Transfer characteristics for different values of the rotation angles θ = 0, 10.5° and 21°, at V_{DS} = 0.3V. Other parameters are: D_{ac} = 3 eV, L_{ext} = 5 nm, L_{OV} = W = 20 nm, T_{BOX} = 1 nm and N_D=4x10^{12} cm^{-2}.

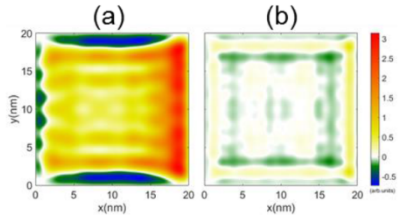

Figure 3. Spatial distribution of the inter-layer tunnelling current in the on state (V_{TG}=0.2V) for misorientation angles of (a) 10.5° (b) and 21°. For large angles, tunnelling is concentrated along the edges of the region of overlap between the two layers.

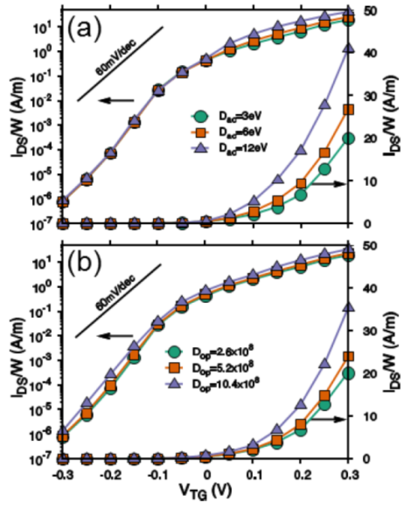

Figure 4. Transfer characteristics for different values of (a) acoustic deformation potential D_{ac} and (b) optical deformation potential D_{op}, with the rotation angles θ = 21°, at V_{DS} = 0.3 V. The optical phonon energy is ħω = 50 meV. Other parameters are as in Fig.2.

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