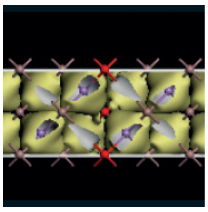

Effects of uniaxial strain on phosphorene tunneling field-effect transistors

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Black phosphorus (BP) field-effect transistors (FETs) show high on/off current ratio and high mobility, thus making BP a promising candidate for future FETs. Theoretical studies predict that single layer BP (phosphorene) tunneling FETs (TFETs) exhibit steep subthreshold swing (SS) and high on-current (I_{ON}). In this work, we perform a first-principles-based quantum transport simulation to investigate the effects of uniaxial strain on phosphorene TFETs.

Phosphorene has a puckered honeycomb structure as shown in Fig. 1(a). We calculate the band structure of strained phosphorene by employing density functional theory (DFT) with the openMX code [1]. The uniaxial strain is imposed along the zigzag direction.

For quantum transport simulation of phosphorene TFETs (Fig.1(c)), the non-orthogonal DFT Hamiltonians are extracted for each strained structure of phosphorene.

The DFT Hamiltonians are reduced in size by the approach in [2] to alleviate the computational cost but without the loss of the accuracy. The Hamiltonians are imported into our in-house quantum transport simulator based on the non-equilibrium Green's function method [2].

The anisotropic band structures of phosphorene are shown in Fig. 2. The unstrained phosphorene has a direct band gap of 0.92 eV. The band gap and effective masses of electron (m_e^*) and hole (m_h^*) are altered by the strain as shown in Fig. 2 and Fig. 3. Especially, it is found that (m_e^*) of both armchair direction (AD) and zigzag direction (ZD) is dramatically changed at the strain of 4%, where the band switching between the first and second conduction bands occurs. Over 8% tensile strain, the band gap at the χ point, which is located between Γ and X points (see Fig. 1(b)), becomes comparable to that at Γ point.

The compressive strain enhances the current of both AD and ZD TFETs due to the band gap narrowing as shown in Fig. 4(a). However, it is difficult for AD and ZD TFETs to be used as low power devices under the compressive strain, because AD TFETs cannot satisfy off-current (I_{OFF}) requirement of 10^{-5} μA/μm for low standby power (LSTP) application and ZD TFETs still show low current level due to heavy m_e^* and m_h^*.

Fig. 4(b) shows the transfer curves of phosphorene TFETs under the tensile strain. Unlike the case of the compressive strain, the band gap increases with the tensile strain of up to 4%, thus deteriorating the current levels of both AD and ZD TFETs. However, over the tensile strain of 4%, the performances of ZD FETs become similar to those of AD TFETs. This is because the band switching drastically reduces m_e^* along ZD but increases m_e^* along AD, changing the tunneling probability.

Fig. 5 shows I_{ON}/I_{OFF} ratio as a function of I_{OFF} for different tensile strain. Under the tensile strain, both AD and ZD TFETs meet I_{OFF} requirement of LSTP devices. Moreover, over 8% strain, they can be operated as high performance (HP) devices with I_{OFF} of 0.1 μA/μm, albeit with low I_{ON}/I_{OFF} ratio. This is because the χ point contributes to the current (see Fig. 2). Nevertheless, Fig. 6 shows that SS is kept below 40 mV/dec under the tensile strain.

In summary, the uniaxial strained phosphorene TFETs are investigated by DFT-based NEGF calculations. We found that as the tensile strain is applied over 4%, the performance of ZD TFETs reaches that of AD TFETs due to the band switching.

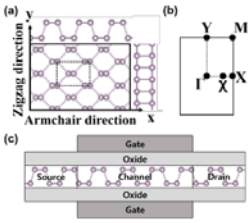

Figure 1. (a) Atomic structure and (b) the first Brillouin zone of phosphorene. Dotted box represents a primitive unit cell of phosphorene. (c) Schematic structure of phosphorene TFET. Channel length and equivalent oxide thickness are 10 and 0.5 nm, respectively. Drain voltage is set to 0.5 V.

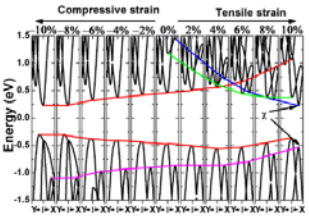

Figure 2. Band structures of phosphorene under uniaxial strain. The band gap decreases with increasing compressive strain, but increases with tensile strain of up to 4%. The band switching between the first and second conduction bands is observed at 4%, after which the band gap decreases. Over 8% tensile strain, the direct band gap at the χ point, which is located on Γ-X valley (see Fig. 1(b)), becomes comparable to that at the Γ point.

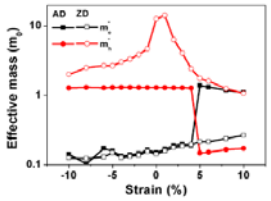

Figure 3. Effective masses of electron (m_e^*) and hole (m_h^*) as a function of strain. m_e^* is dramatically changed at 4% tensile strain due to the band switching (see Fig. 2).

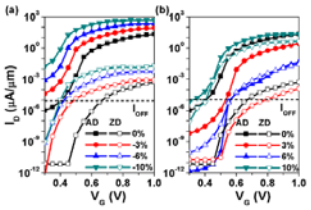

Figure 4. Transfer characteristics of phosphorene TFETs under compressive strain. I_{OFF} is 10^{-5} μA/μm for LSTP devices. The current levels of AD and ZD TFETs increase with the compressive strain. Below 4% strain, the current levels of AD and ZD TEFTs decrease with increasing tensile strain. Over 4% strain, the current levels of ZD TFETs become comparable to those of AD TFETs.

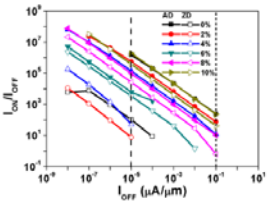

Figure 5. I_{ON}/I_{OFF} as function of I_{OFF} for different tensile strain. Dashed and short-dashed lines represent LSTP and HP applications, respectively.

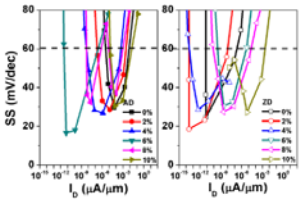

Figure 6. SS versus I_D. Under the tensile strain, SS is kept lower than 40 mV/dec.

[1] T. Ozaki *et al.*, *Phys. Rev. B*, 72, 045121 (2005).
[2] M. Shin *et al.*, *J. Appl. Phys.*, 119, 154505, (2016).