Student Paper

Strain Response of Monolayer MoS_2 under Ballistic Limit

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Two-dimensional (2-D) materials are perfect channels for ultra thin body (UTB) device due to the perfect electrostatic control. Graphene has been widely believed as a promising candidate. However, its gapless nature limits its potential application as logic transistors. To overcome the shortage of graphene-based transistors, 2-D monolayer transition metal dichalcogenides (TMD) with intrinsic bandgap (1eV~2eV) have drawn much attention. MoS_2 is expected to be one of the promising candidates among all TMD materials for the channels of UTB FETs [1][2]. Strain technology is in fact responsible for an alteration of the band structure in silicon to enhance the device performance [3]. With the appropriate strain engineering on TMD materials, the high performance transistor could be achieved.

The periodic atomic structure of MoS_2 is shown in **Fig.1**. Three strain conditions are applied: 1) isotropic tensile strain, 2) uniaxial tensile strain along armchair direction (x-direction), and 3) uniaxial tensile strain along zigzag direction (y-direction). The CASTEP simulation package was employed to perform density functional theory calculations with the approximation of the generalized gradient corrected functional used for the exchange-correlation potential. The cutoff energy for the wave-function expansion is set to 450 eV, and a mesh of 18 × 18 × 1 points in k-space is used for 2-D Brillouin-zone integrations. To perform the mechanical response in the elastic range of monolayer MoS_2, the in-plane Poisson's ratio of 0.21 and out-of-plane of 0.27 [4].

The out-of-plane S-Mo-S bond angle at the stress-free state is 81.1°. **Fig.2** shows the variation of such S-Mo-S bond angle as a function of the applied tensile strain under different strain paths. It can be seen that the S-Mo-S bond angle decreases the most for isotropic tension and the least for uniaxial tension along zigzag direction.

Fig.3 shows the bandgap shift with increasing tensile strain. At the strain larger than 1%, the bandgap becomes indirect. The bandgap reduces dramatically under isotropic tensile strain and the both uniaxial strain conditions have less reduction of bandgap. The lowest conduction band is K valley with tensile strain. The electron effective mass in K-valley for the unstrained monolayer MoS_2 is $0.49m_0$ along Γ-K direction and has similar value on its orthogonal direction. In **Fig.4**, m_x and m_y decrease with the same magnitude under isotropic strain and have symmetry on K and K' valley. Under the uniaxial strain, the original crystal symmetry is broken. As a result, K' valley becomes no longer equivalent to K valley. In armchair tensile strain, the constant-energy contours on K point become elliptic. The major axis is along the Γ-K direction (m_y) and minor axis is on its orthogonal direction (m_x). The zigzag strain has the opposite trend (**Fig.5**).

The top-of-the-barrier ballistic model is used to solve the current density (**Fig.6**) [6]. The density of states and velocity of the carrier are main factors determining the magnitude of current density. The ballistic current with 3% tensile armchair has largest current density due to larger density of states mass (m_{DOS}) and smaller mass along the current flow (m_t) than isotropic condition (**Fig.7**). In contrast, the current of 3% zigzag strain is smaller than 3% isotropic strain due to larger m_t of K' valleys. **Fig.8** shows the enhancement of all strain condition form 1% to 3%. Notice that there is a suddenly drop under 1% zigzag strain due to the large K' effective mass.

In summary, response of monolayer MoS_2 under appropriate strain condition can enhance current density in ballistic regime. The anisotropic energy contour between Γ-K direction and its orthogonal direction under uniaxial strain cause the improvement of the ballistic current of monolayer MoS_2. The current enhancement of armchair strain is 22% larger than unstrain for the 3% uniaxial tension.

Acknowledgement

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References

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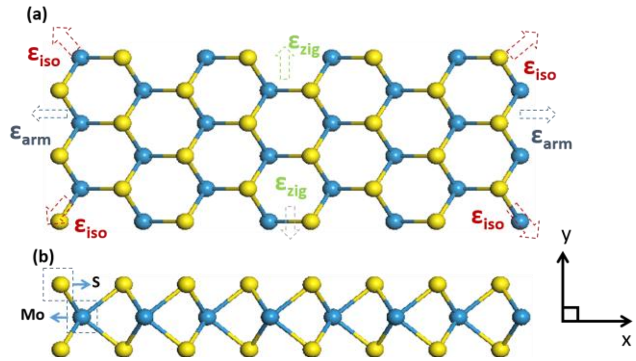

Fig.1 (a) Top view of crystal structure of monolayer MoS_2. (b) Side view of the monolayer. Mo atom layer is sandwiched between two S atom layers.

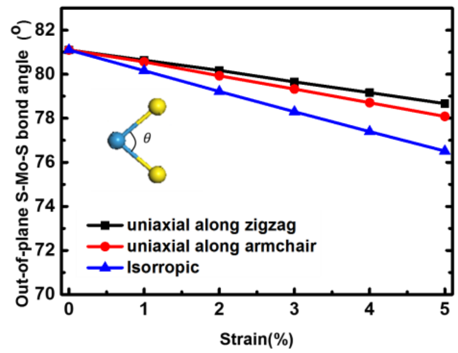

Fig.2 The variation of out-of-plane Mo-S bond angle in different strain, the angle decrease of biaxial is largest and that of zigzag is smallest

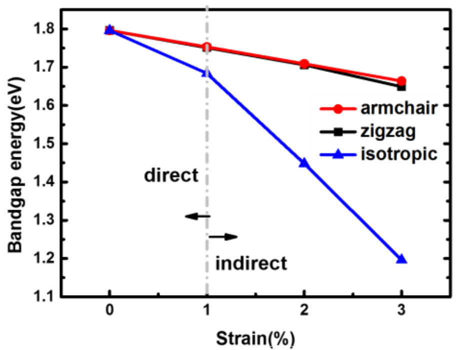

Fig.3 Calculated bandgap shifts under different strain conditions.

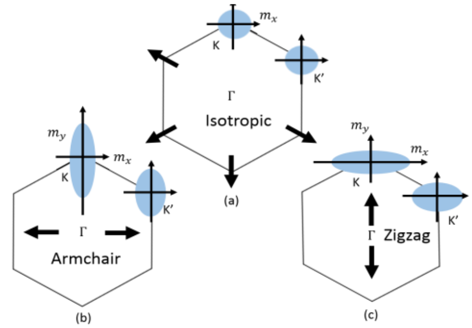

Fig.4 Schematic diagram of the constant-energy contours in the conduction band for (a) Isotropic strain (b) armchair strain and(c) zigzag strain.

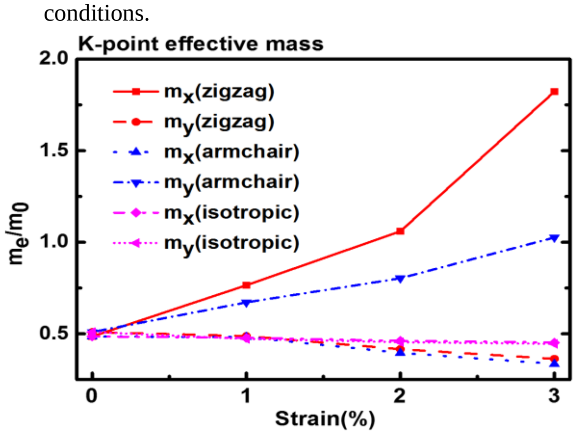

Fig.5 The electron effective mass with different tensile strain conditions.

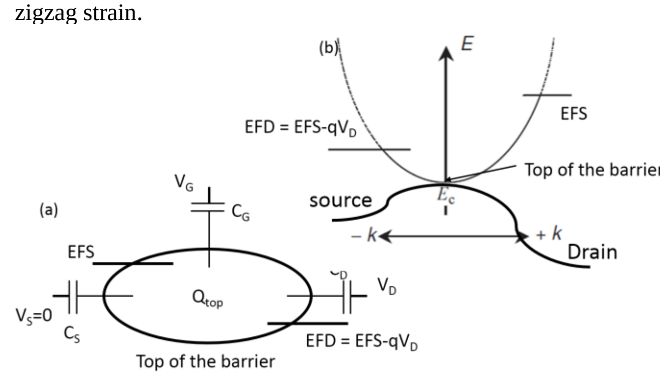

Fig.6 (a) Two-dimensional circuit model for ballistic transistors (b) The energy on the top of the barrier. EFS and EFD are the Fermi level of source and drain respectively

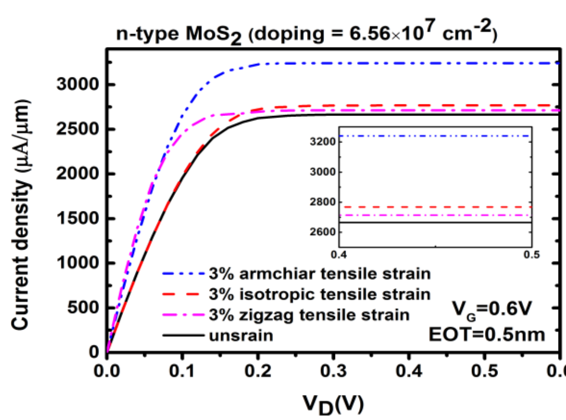

Fig.7 The output characteristics for current in strain condition, the current direction of two uniaxial strain are along their strain direction.

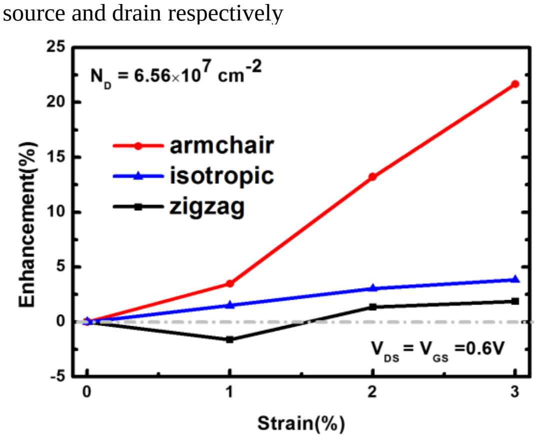

Fig.8 The ballistic enhancement of three strain with different Engineering strain conditions.