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Simulation Investigation of Strained Black Phosphorus p-n Photodetector for Middle Infrared Range

Siqing Zhang, Yan Liu, Genquan Han, Jincheng Zhang and Yue Hao

Wide Bandgap Semiconductor Technology Disciplines State Key Laboratory, Xidian University, Xi'an, 710071,
Corresponding: Genquan Han(e-mail:hangenquan@ieee.org）

Abstract

In this paper, we design a uniaxially strained black phosphorus (BP) photodetector with p-n structure. Different strains applied in the zigzag or armchair direction can effectively tune the direct band gap of 5-layer of BP. The strain effect on the band structure of BP is investigated using first-principles method based on density functional theory. The cut-off wavelength of strained 5-layer of BP p-n photodetector is extended to about 8 μm, which means that the strained black phosphorus p-n photodetector provided a new approach for middle-infrared range photoelectric devices.

1. Introduction

As we all know, the commonly used materials for photodetectors in infrared band mainly refer to PbS, InGaAs, PbSe, and InSb. However, none of them can fully cover the whole mid-infrared (MIR) range. In recent years, two dimensional materials including graphene, transition metal dichalcogenides, and black phosphorus (BP) have been regarded as the future materials of new photoelectric devices. As for BP, it owns direct band gap, which can be tuned from 0.3 eV to 2 eV by changing the number of layers and the strain applied to it. Due to this remarkable property, BP has attracted a lot of interest for the extensive applications for the MIR photonic devices.

In this paper, we design and simulate a strained BP-based p-n photodetector. Comparative study on strain effect of black phosphorus and energy structures under different strains along zigzag or armchair direction are carried out. The optimized cut-off wavelength reaches 8 μm at ε_y =-5%, which means that the spectral window of BP-based photodetector can be extended into MIR range.

2. Device Design

Fig.1. (a) shows 3D device structure of the strained BP p-n photodetector. By tensing and compressing PDMS (polydimysiloxane), we can apply different strains to 5-layer of BP along zigzag and armchair direction respectively. Among 5-layer of BP, 2 layers are p-type after doping MoO_3 and 3 layers are n-type after doping Cs_2CO_3 to form p-n junction. For convenience, we define armchair direction as x direction and zigzag direction as y direction.

3. Strain effect of black phosphorus

In this work, 5-layer of BP was chosen to evaluate strain effect on the band structure of black phosphorus. The simulation of strain effect along armchair and zigzag directions were both performed by Nanodcal Software. As shown in Fig.1. (b), phosphorus atoms in BP are arranged forming a puckered honeycomb lattice, which includes two different directions: the zigzag (parallel to the atomic ridges) and the armchair (perpendicular to the ridges)[1].

Fig. 2 shows the tangible deformation with different strain in armchair and zigzag directions. The atomic distance and the band angle between phosphorus atoms in armchair direction are shorten at ε_x = -20% and vice versa which can be seen in Fig. 2 (a-c). Along the zigzag direction, the distance between phosphorus atoms follows the same law as shown in Fig. 2 (d-f).

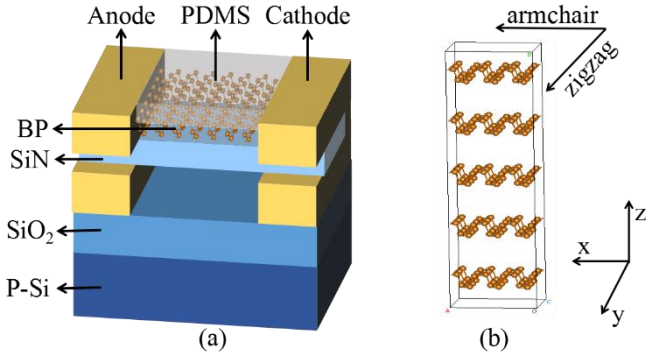

Fig.1. (a) Schematic diagram of a BP-based p-n photodetector. (b) Crystal structure of 5-layer of BP.

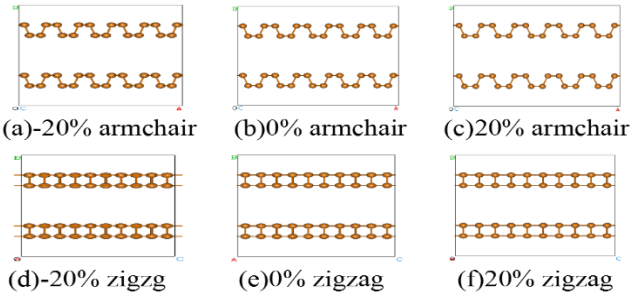

Fig. 2. Sketch maps of strain effect along armchair and zigzag directions.

4. Results and Discussion

Due to the reduced-dimensional structures which can sustain much larger strain than bulk crystals, the band structure tends towards a more symmetric state along with changing band structure and energy band gap at the same time. Our calculated band gap for relaxed 5-layer of BP is 0.498 eV at Γ point roughly coinciding with theoretical value[2].

Fig.3. indicates that at ε_x = 3% and ε_y = 3% respectively, the energy band gap is raised up to 0.724 eV and 0.697 eV at Γ point. Regarding the compressed BP at ε_x = -3% and ε_y =

-3%, the energy band gap of black phosphorus drops to 0.253 eV and 0.294 eV at Γ point. As the compressive stain reaches ε_x = -9% and ε_y = -9% respectively, either in armchair or zigzag direction valence band maximum (VBM) clings to conduction band minimum (CBM), which means the energy band gap equals to zero.

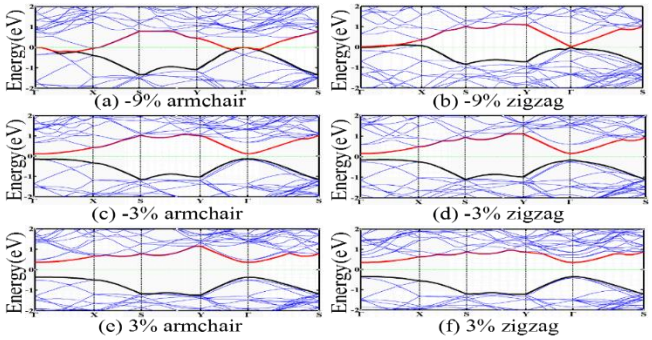

Fig.3. Energy structures of the 5-layer BP at (a) ε_x = -9%, (b) ε_y = -9%, (c) ε_x = -3%, (d) ε_y = -3%, (e) ε_x = 3%, and (f) ε_y = 3%.

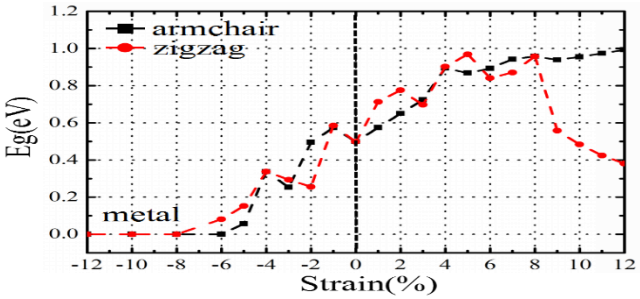

Fig.4. Energy band gap E_g versus the applied uniaxial strain for 5-layer BP.

Fig.4. reveals the variation of energy band gap under different strains for 5-layer of BP. Firstly, the band gap along two directions are both increase in general for the tensile strain varying from 0% to 8%, while after ε_y = 8%, the band gap begins to drop down at zigzag direction. Secondly, just like a direct-indirect-direct transition of 2D phosphorene when axial strain is applied[3], the band gap of 5-layer first transitions to indirect and then experiences a semiconductor-metal transition (SMT) with compression increasing. When ε< -6%, a SMT appears along two directions, which can be seen from the plateau in Fig.4. As for ε_y = -5%, Eg is 0.152 eV which is much smaller than that of relaxed BP. This remarkable decrease signifies that BP-based photodetector can cover MIR. When ε_y = -6% and ε_x= -5%, Eg reaches 0.0816 eV and 0.057 eV respectively and the band structures both change into indirect band, that is to say, the conduction band minimum (CBM) and the valence band maximum (VBM) are at different k-points. Owing to the indirect light absorption which must consider phonon for satisfying momentum conservation, the indirect absorption coefficient α_2 in Eq. (2) and Eq. (3) is smaller than direct absorption coefficient α_2 in Eq. (1) by almost three orders of magnitude. So the optimized Eg is defined as 0.152 eV for maximal light absorption efficiency of the BP-based photodetector.

$$\alpha_1(\hbar\omega) = \frac{\alpha_b}{(2\pi)^2}\left(\frac{2m_r}{\hbar^2}\right)(\hbar\omega - E_g)^{\frac{1}{2}} \quad (1)$$

Here, E_g is the direct bandgap of semiconductor materials, $\hbar$ is the Planck constant, and m_r is the reduced mass of semiconducting materials.

$$\alpha_2(\hbar\omega) = C_1(\hbar\omega + E_q - E_g)^2 N_q(T) \quad (2)$$

$$\text{where } C_1 = \frac{4\pi^2 e^2 C}{m^2 n^2 V_g \omega}\frac{1}{8(2\pi)^3}\left(\frac{2m_c^*}{\hbar^2}\right)^{\frac{3}{2}}\left(\frac{2m_v^*}{\hbar^2}\right)^{\frac{3}{2}} \quad (3)$$

Here, E_q is phonon energy, $N_q(T)$ is the number of phonons, V_g is photon flow velocity.

Fig. 5 shows us the relation between the direct absorption coefficient α_1 and wavelength λ for relaxed and strained 5-layer BP. First we focus on the cut-off wavelength. For the relaxed 5-layer BP, the cut-off wavelength is about 2.49 μm, When ε_y is -5%, the cut-off wavelength for absorption spectra red shifts and reaches 8 μm. Second as for the direct absorption coefficient α_1 under strain, it decreases owning to the reduction of reduced quality m_r, which can be obtained by the change of the curvature of the energy band under strain.

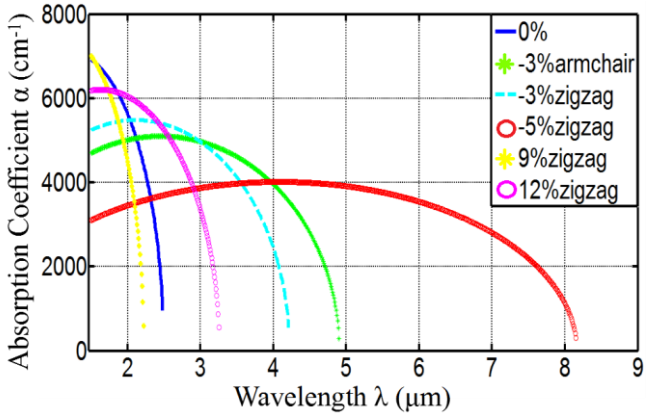

Fig.5. Calculated absorption spectra for relaxed and strained 5-layer BP p-n junction photodetector.

5. Conclusions

In order to investigate strain effect on black phosphorus p-n junction photodetector, the band structures of 5-layer BP along different directions at different strain were simulated. Owning to valence band maximum (VBM) increases and conduction band minimum (CBM) decreases at Γ point under compression, band gap therefore shrinks and the cut-off wavelength extends to 8μm, which can pave a new way for BP-based photodetector in the middle-infrared range (MIR).

References

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