Effect of shear strain on band structure and electrical properties of phosphorene

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Abstract

We present an ab-initio investigation of effects of shear strain on band structure and electrical properties of 2D phosphorene. We carried out DFT calculations to determine the shear stress as a function of shear strain and found the monolayer phosphorene has ultimate strength at shear strain 30% and 35% in armchair and zigzag directions, respectively, and it was also found that the monolayer extends in z direction on applying shear strain in both directions. Additionally we derived band structures of phosphorene and effective electron and hole masses along both directions under shear strain and have shown that band gap in phosphorene decreases along both directions and that phosphorene shows a semi-metal nature on applying shear strain of magnitude 30% in both directions. The electrical conductivity of phosphorene was estimated by effective mass along zigzag and armchair directions and it is shown that the electrical conductivity is far higher along armchair direction and that, with increasing shear strain, conductivity increases along armchair, up to ultimate strength, and zigzag directions.

References

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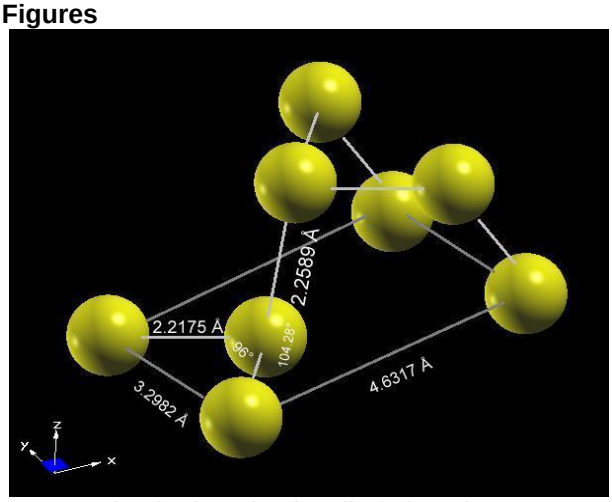
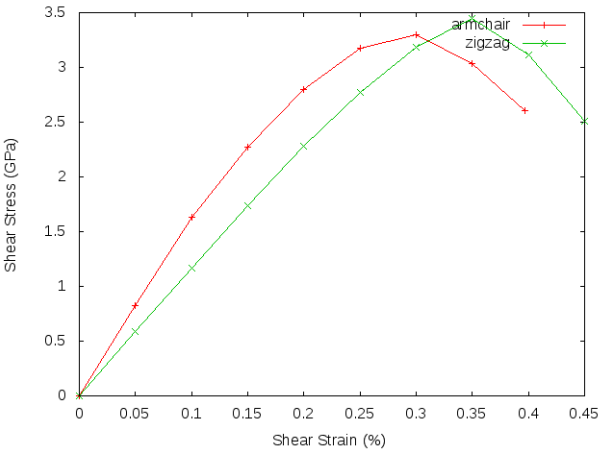
[2] Li, Likai, et al. **Nature nanotechnology** (2014).
[3] Rodin, A. S., A. Carvalho, and AH Castro Neto. **Physical review letters** 112.17 (2014): 176801.
[4] Giannozzi, Paolo, et al. **Journal of Physics: Condensed Matter** 21.39 (2009): 395502.

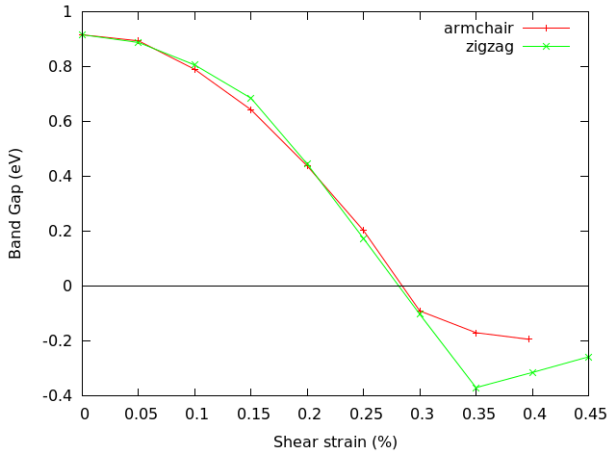
Figures



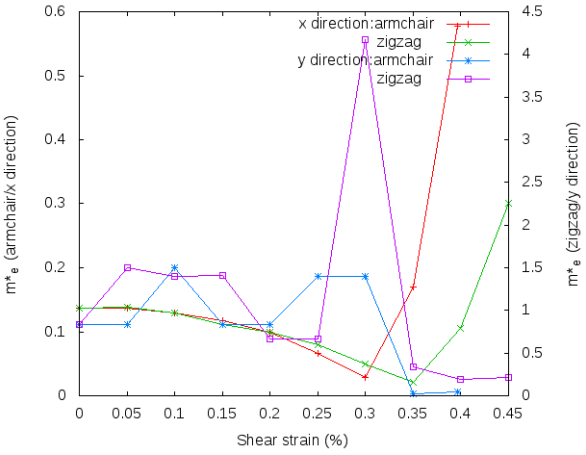
Derived relaxed unit cell of phosphorene



Shear Stress (GPa) v/s Shear Strain (%)



Band gap (eV) v/s Shear Strain (%)



Effective electron mass v/s Shear Strain (%)