A Study of the Electronic Properties of Materials for a 2D Transistor via Computer Simulation

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Introduction

In this age of rapid technological innovation, there is pressure to maximize device efficiency while minimizing size. Transistors, a key component of modern electronics, prove to be one of the biggest challenges. They are made up of three integral parts: a semiconductor, conductor, and insulator. Recently, scientists have moved to using two dimensional (2D) materials to create smaller transistors. These materials are atomically thin in one direction and also offer the possibility of creating a flexible and transparent device[1].

Objectives

- Evaluate the suitability of three materials for the fabrication of a 2D transistor by studying their electronic properties in terms of conductivity, band gap and transparency
- Evaluate the suitability of these materials for a flexible and transparent transistor by studying how their electronic properties are effected by strain and compression and by calculating their reflectivity

Methods

Define and visualize atomic structure with VESTA (Fig. 1) → Relax structure using Vienna Ab Initio Simulation Package (VASP) → Calculate the dielectric constant with VASP → Repeat process with compressed and strained structures → Calculate the band gap, conductivity, and reflectivity for all structures → Analyze the data to evaluate the material's performance

Equations

Reflectivity[2]:

$$1)\quad R = \frac{(1-n)^2+k^2}{(1+n)^2+k^2}, \quad k = \sqrt{\frac{|\varepsilon| - \varepsilon_1}{2}}, \quad n = \sqrt{\frac{|\varepsilon| + \varepsilon_1}{2}}$$

Conductivity[2]:

$$2)\quad \sigma = \frac{\omega \varepsilon_2}{4\Pi}, \quad \omega = \frac{E}{\hbar}$$

n – index no. fraction
ε – dielectric constant
k – extinction coefficient
ε_1 – real part of dielectric constant
R – reflectivity
E - energy
$\hbar$(plank constant divided by 2π) $= 4.13^{-15}$
ω – frequency
σ – conductivity
ε_2 – imaginary part of dielectric constant

Materials

a) b) c)

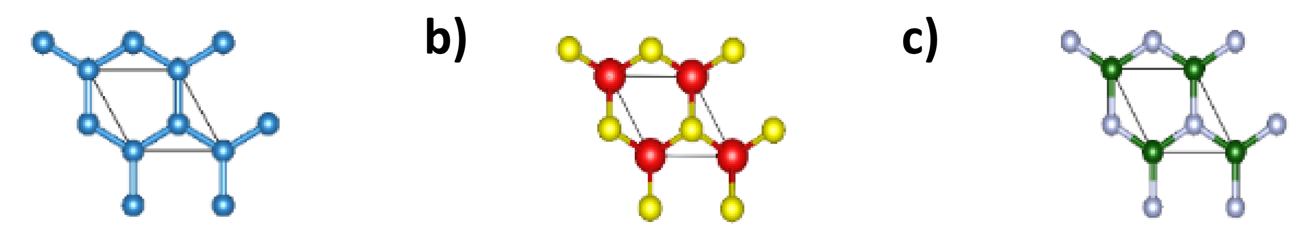

Figure 1 - a) unit cells of Graphene b) Molybdenum Disulfide (MoS2) and c) Hexagonal Boron Nitride (h-BN)

Results and Discussion

Band Gaps

- Graphene is consistently metallic under all values of strain
- MoS_2 has a medium-sized band gap which decreases under strain
- The reduction of the MoS_2's band gap energy under positive strain is significant
- H-BN has large band gap which decreases slightly under compression and strain

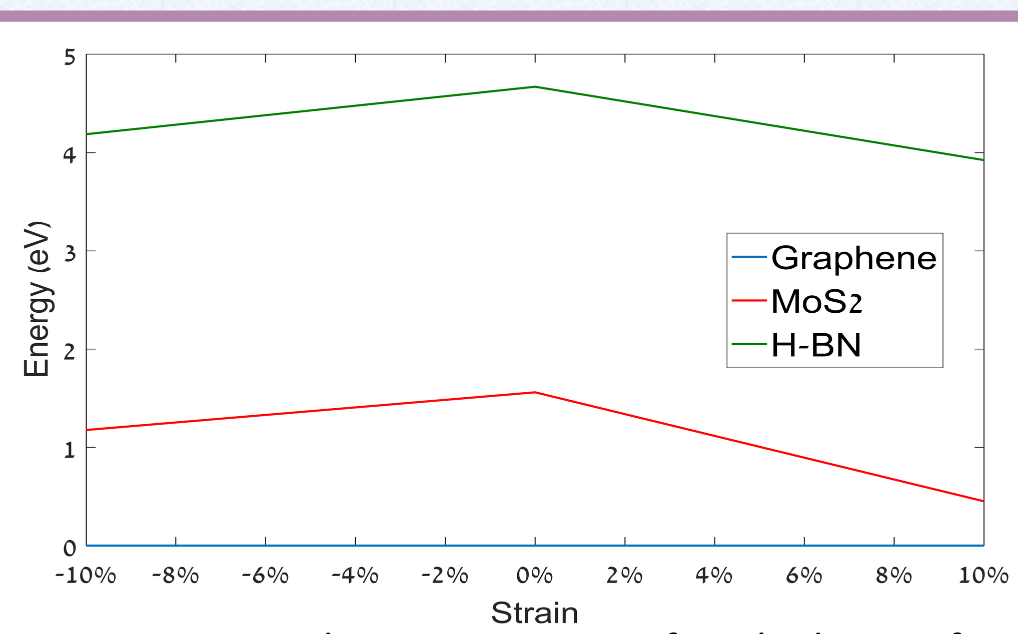

Figure 2 – Band Gap vs. percent of applied strain for Graphene (blue) MoS_2 (red) and H-BN (green)

Reflectivity

- Graphene is fairly transparent and its reflectivity is not significantly affected by strain or compression (Fig. 3)
- MoS_2 is not very transparent in its relaxed state, however this improves under strain and compression (Fig. 4)
- H-BN is consistently transparent under all values of strain, with the reflectivity increasing almost linearly across the visible spectrum (Fig. 5)

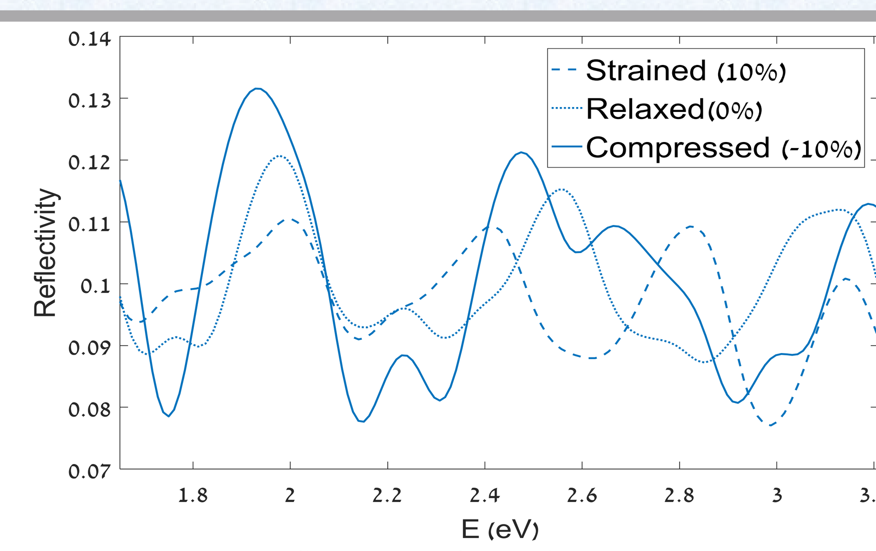

Figure 3 – Reflectivity of Graphene vs. Energy of incident light in the visible spectrum

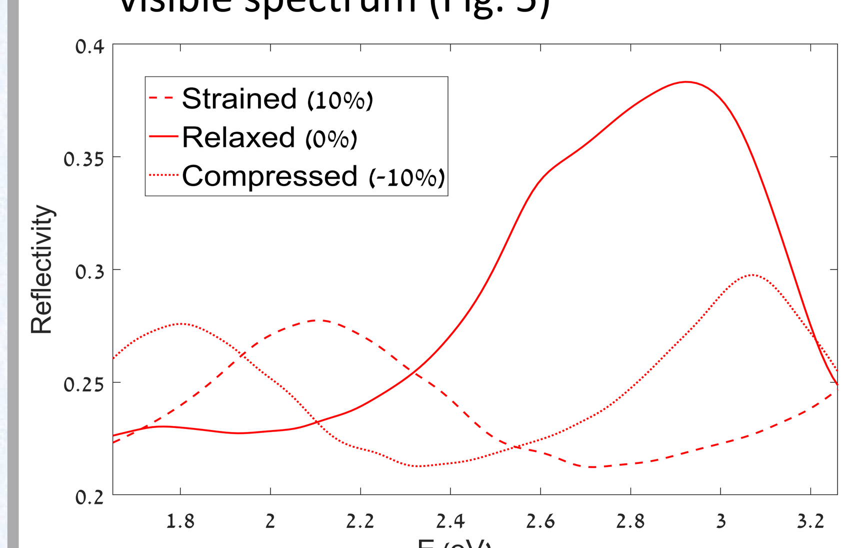

Figure 4 – Reflectivity of MoS_2 vs. Energy of incident light in the visible spectrum

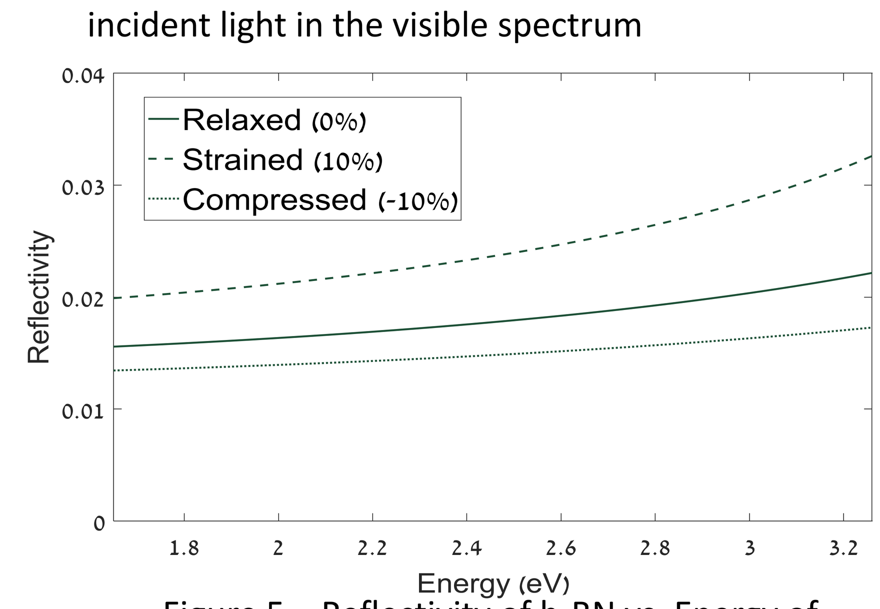

Figure 5 – Reflectivity of h-BN vs. Energy of incident light in the visible spectrum

Conductivity

- Graphene is the only material that is conductive without additional energy (Fig. 6)
- MoS_2 becomes conductive around the energy of its band gap and quickly becomes the most conductive of the three materials (Fig. 6)
- H-BN requires the most energy to become conductive and has the lowest values of conductivity (Fig. 6)
- The conductivity of Graphene and MoS_2 are not significantly affected by strain or compression (Figs. 7 and 8)
- H-BN because more conductive under strain and less conductive under compression (Fig. 9)

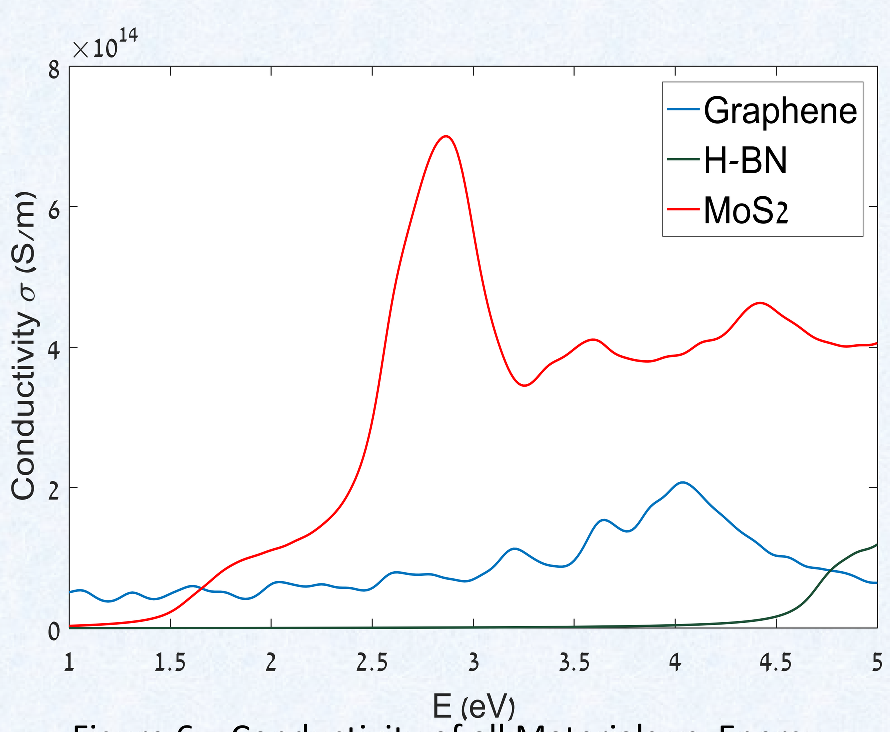

Figure 6 – Conductivity of all Materials vs. Energy (-10%, 0%, 10% strain)

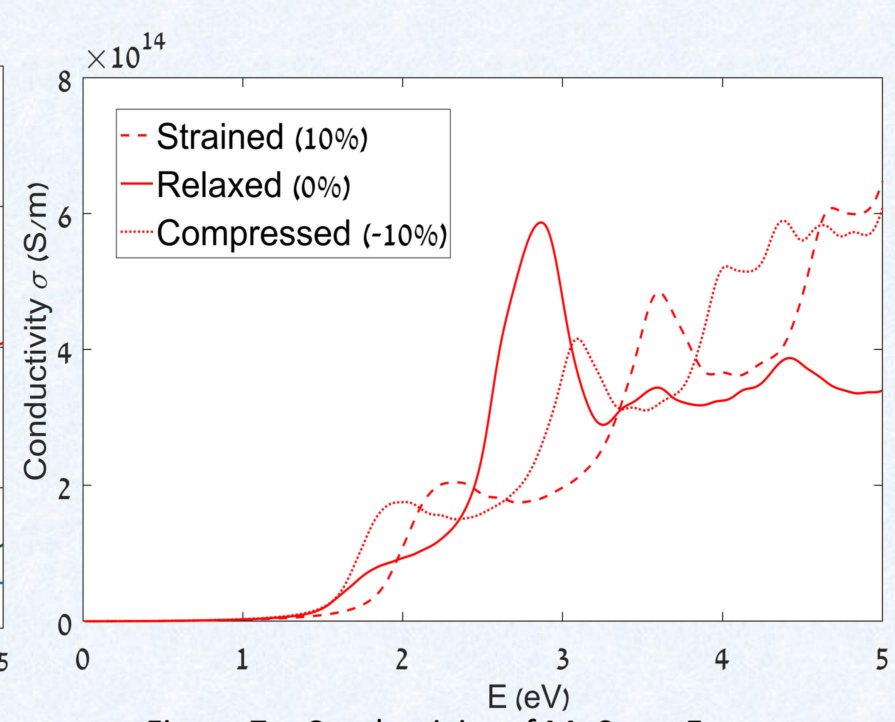

Figure 7 – Conductivity of MoS_2 vs. Energy (-10%, 0%, 10% strain)

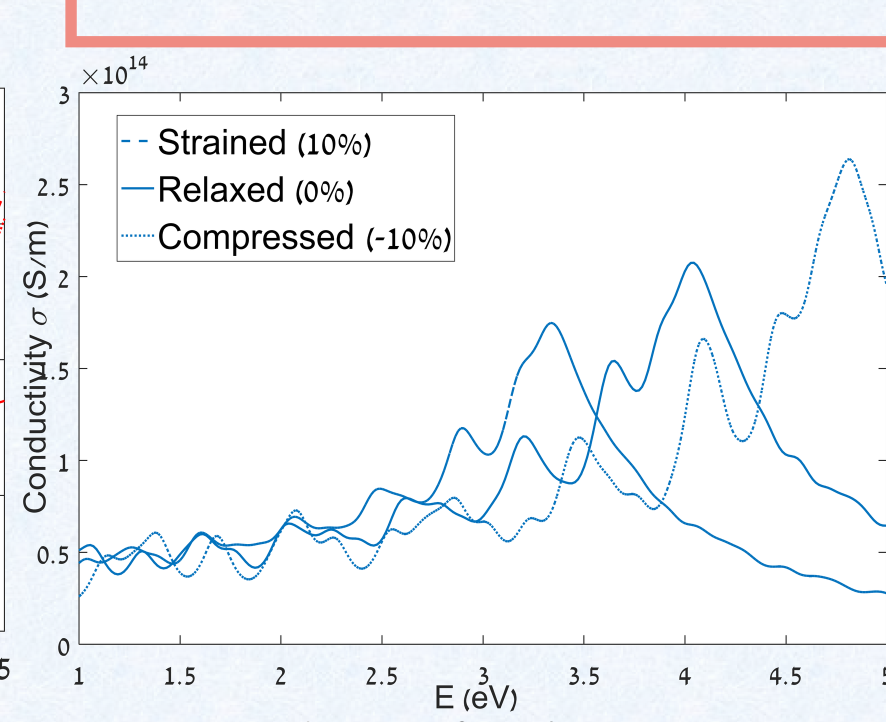

Figure 8 – Conductivity of Graphene vs. Energy (-10%, 0%, 10% strain)

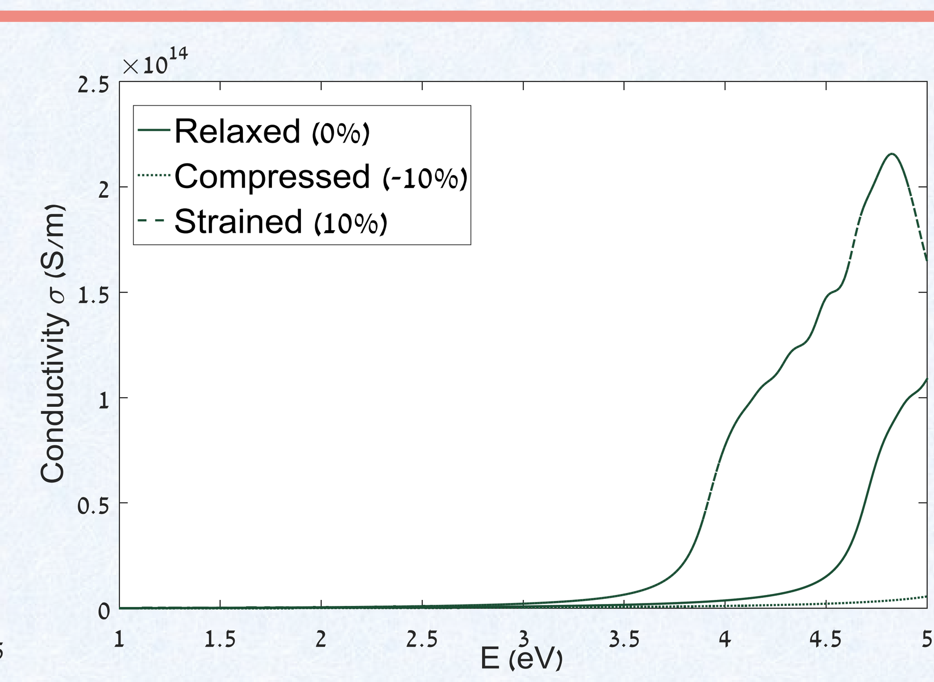

Figure 9 - Conductivity of H-BN vs. Energy (-10%,0%,10% strain)

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References

1. Roy, Tania, et al. "Field-effect transistors built from all two-dimensional material components." *ACS nano* 8.6 (2014): 6259-6264.
2. Tanner, David B. "Optical effects in solids." Department of Physics, University of Florida, USA (2013).

Conclusions

- Without the application of external strain, all the materials exhibit good electronic qualities.
- Graphene is a good candidate material for the conductor in a 2D flexible and transparent transistor, with excellent electronic properties that are not affected by strain and compression
- H-BN does not perform as well, becoming slightly more conductive under strain, but is still a good candidate material for the insulator in a 2D flexible and transparent transistor
- MoS_2 is not very transparent in its relaxed states, and also becomes much more conductive under strain which would make it an ineffective material to use when creating a flexible and transparent device
- In general, there is a trend that the band gap decreases as strain or compression is applied which could be indicative of a weakening of the bonds in the material