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AUGUST 31 - SEPTEMBER 03, 2021 ● ONLINE

TECHNISCHE UNIVERSITÄT DRESDEN

complex nano materials

Electronic and Thermal Transport in Black Phosphorene tunned by Grain Boundaries and Strain

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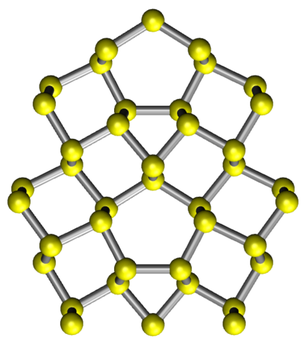
INTRODUCTION

Grain Boundaries in 2D materials

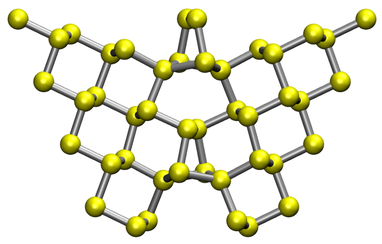
Grain boundaries are a lattice defect type that is found commonly after the synthesis of 2D materials due to the growing and merging of two grains with different nuclear sites and lattice orientations. This type of defects influences the mechanical and electronic properties of the materials. [1,2]

Aim

Understand the effect of the grain boundaries into the electronic and lattice properties of phosphorene in order to engineer grain boundaries to tune transport properties of low dimensional systems.



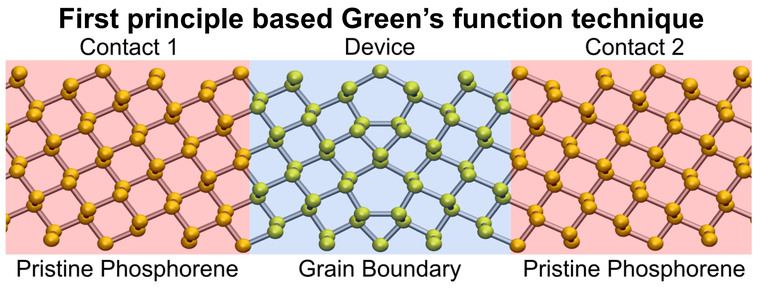
GB 1



GB 2

METHODOLOGY

First principle based Green's function technique



Device Green's function:

$$G = (EI - H - \Sigma_L^r - \Sigma_R^r)^{-1}$$

$$G = \left(\omega^2 I - K - \Sigma_L^r - \Sigma_R^r\right)^{-1}$$

DFTB — Density Functional based Tight Binding method

Electronic Transmission function:

$$\tau_{el}(E) = \mathrm{Trace}\,(G^r \Gamma_L G^a \Gamma_R)$$

Phonon Transmission function:

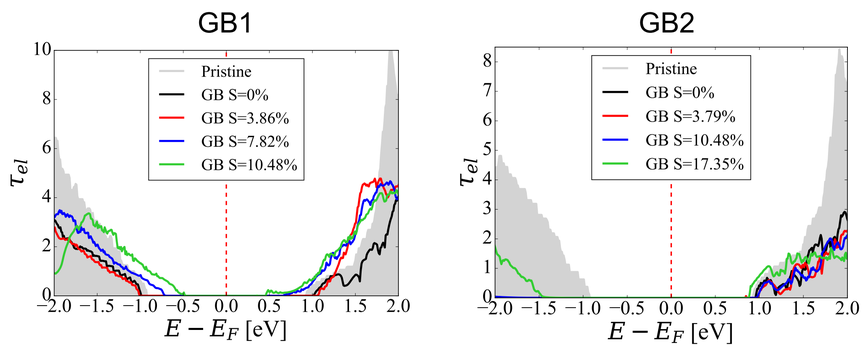
$$\tau_{ph}(\omega) = \mathrm{Trace}\,(G^r \Gamma_L G^a \Gamma_R)$$

Thermal Conductance:

$$\kappa_{\mathrm{ph}} = \frac{1}{2\pi}\int_0^\infty \mathrm{d}\omega\ (\hbar\omega)\ \frac{\mathrm{d}N_{\mathrm{B}}}{\mathrm{d}T}\ \tau_{\mathrm{ph}}(\omega)$$

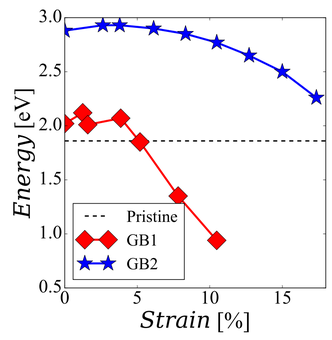
RESULTS

Electronic Transmission



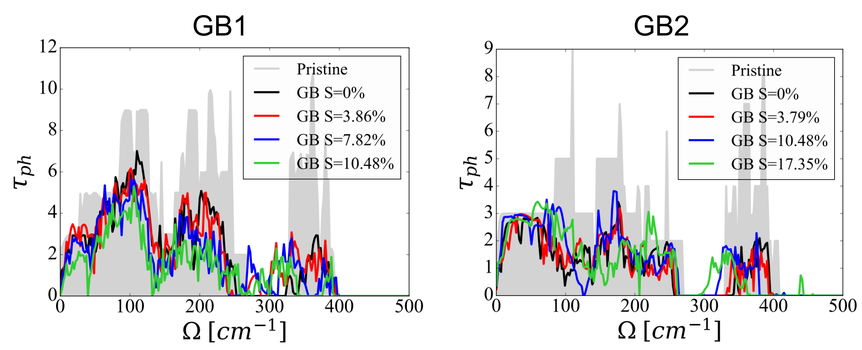
Incorporation of GB's decreases the electronic transmission in the system. Strain enhances electronic transmission, extending the transmission at regions above and below the HOMO and LUMO.

Band gap of GBs under strain



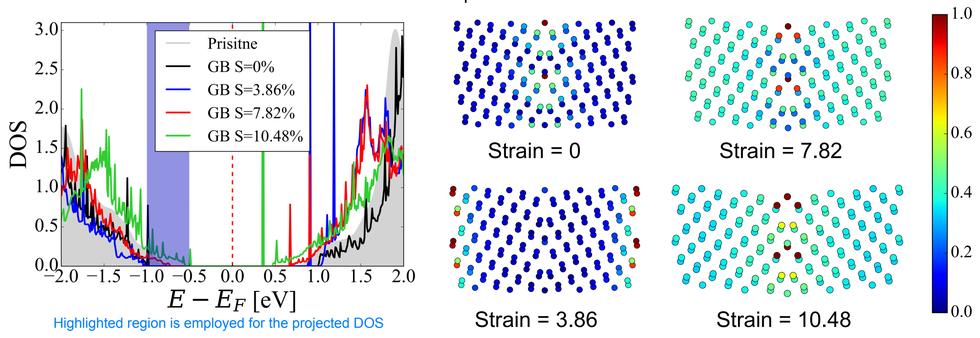
GB's increases the band gap.
Strain decreases the band gap.

Phonon Transmission



GB's decreases the phonon transmission in the whole spectrum.
Strain induce the formation of phonon band gaps as well the emergence of channels where no transmission was present.

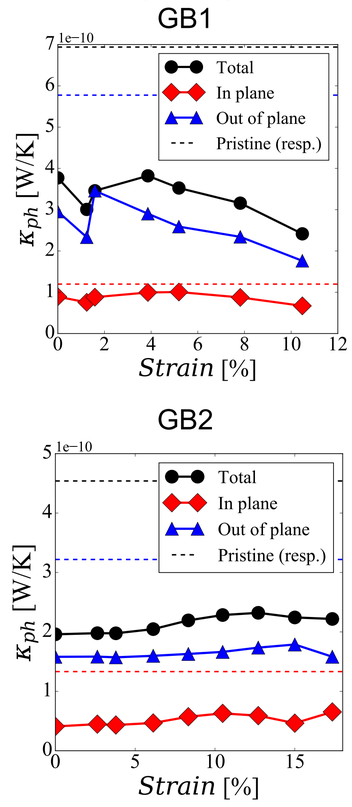
Projection of electronic DOS in GB1



The DOS at energy regions below the Fermi level are dominated by the GB. The strain enhance the DOS of the whole system, but mainly the GB region.

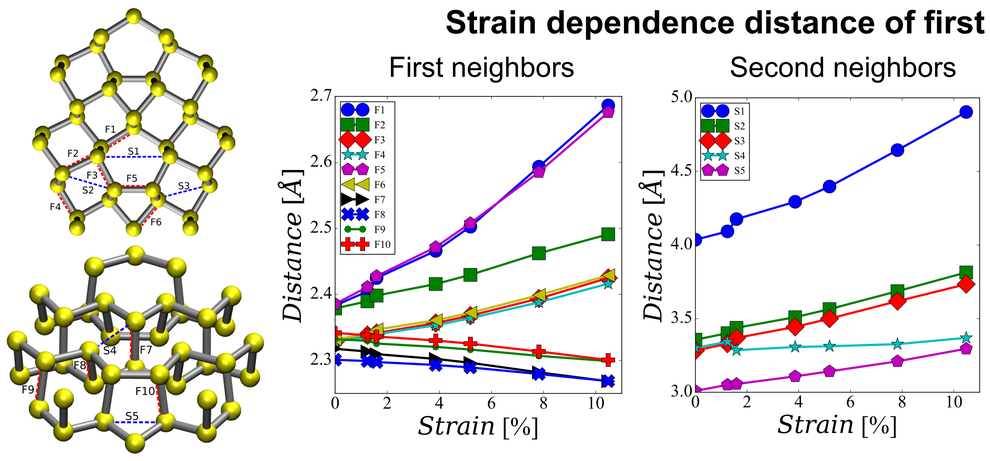
At energy regions above the Fermi level there is an enhancement of DOS by atoms near the contacts by increasing the strain, but the DOS of the GB decreases.

Thermal Conductance (300K)



GB's drastically decreases thermal conductance ~50%.
Strain further decreases thermal conductance in GB1, but not in GB2.

Strain dependence distance of first and second neighbors around the GB



Bond distance between in-plane 1st neighbor atoms increase proportionally with strain, which correlated with the enhancement in the electronic transmission.

The bond distance between some 1st neighbors decrease gradually, and other atoms remain almost constant,except when strain > 12%, when they exponentially increase. This causes fluctuation in the electronic transmission at different energies.

CONCLUSIONS

In this research it has been found that grain boundaries and strain can be used to tune the electronic and phonon transport properties of phosphorene.

Compared with the pristine system, the electronic and thermal transmission decreases with the grain boundaries due to the scattering in the interface, on the other hand, the strain modify the molecular geometry which enhances or decreases the density of states at certain regions, as well as it also modifies the electronic and thermal transmission.

The decrease in the electronic band gap as well as the linear correlation between the strain and the electronic transmission makes the phosphorene with GB1 more suitable for electronic applications under low strain (<10%).

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REFERENCES

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[2] Medrano Sandonas, L., Gutierrez, R., Pecchia A., Seifert G., & Cuniberti, G. *Physical Cemistry Chemical Physics*, 2 (2017).

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