Bandgap Observations in Different Crystal Structures via Ab-Initio and DFT Calculations

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Objective & Research Question:

Utilize VASP to simulate and predict light emission from SiGe and SiC alloys with varying crystal structures and induced isotropic strain. The ultimate goal is to analyze potential direct band gaps and maximize efficiency in VASP computations.

Background:

- A digitized world means an increase in data, which requires optimized data transmission. This task is currently done through light (optical fibers) which are not constrained by the limitations of electrical currents.
- Efficient light emission from Silicon provides immense breakthroughs in optical circuitry.
- Transistors communicating via optical means instead of electrical currents can revolutionize the speed and operating power of semiconductor devices.
- Bulk Silicon has no direct bandgap and is unable to emit and absorb light.

Methods:

- Utilize VASP to reveal potential direct band gaps at different k-points in SiGe and SiC with hexagonally close packed and triclinic (TRI1a) crystal structure.
- Compute again with isotropic expansion of factor 1.05.

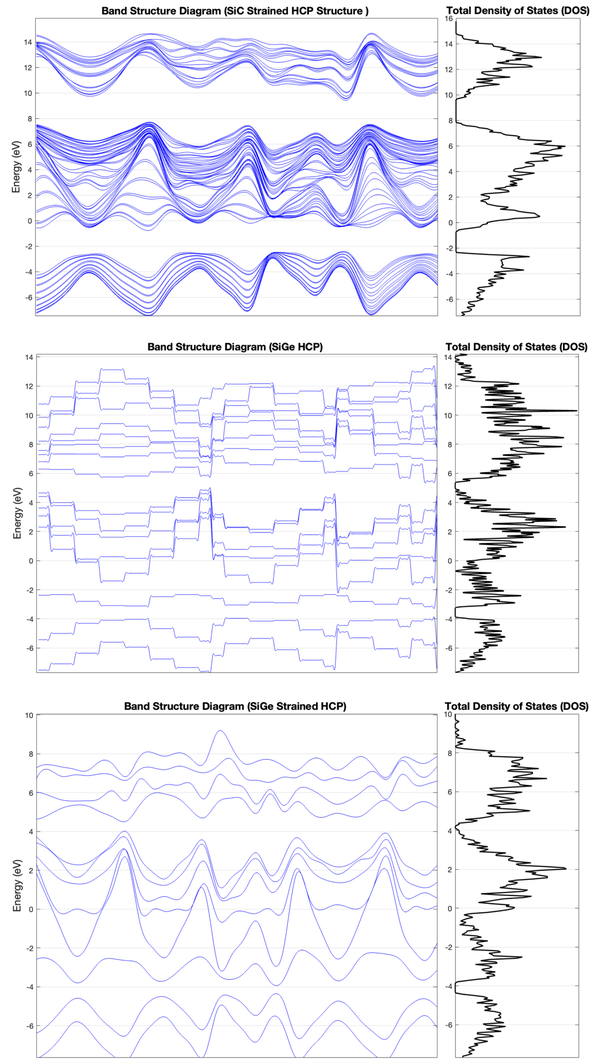

Fig. 1 DOS and band structures of different alloys

Results/Future Goals:

- Indirect band gap is strictly observed in all SiC alloys regardless of strain and different crystal structure. Although, strain does decrease the size of the band gap.
- Computations for Hexagonal SiGe yielded a direct band gap at the Γ-point, which replicates findings by Fadaly et al.
- Smaller eV band gap is seen with introduction of strain in Hexagonal SiGe alloys, potentially hinting to more light emission. Further calculations and tests have to be conducted for verification of findings.
- My future goal is to continue research in this topic. I want to use machine learning models to calculate band gaps in non-bravais and unique crystal structures.

Acknowledgements/ References:

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