Strain induced direct-indirect transition in III-V semiconductor materials from *ab-initio* approach

Badal Mondal and Ralf Tonner
Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie
Universität Leipzig
Linnéstraße 2, 04103 Leipzig
Email: badal.mondal@studserv.uni-leipzig.de

UNIVERSITÄT LEIPZIG | Philipps Universität Marburg | GRK 1782 Functionalization of Semiconductors

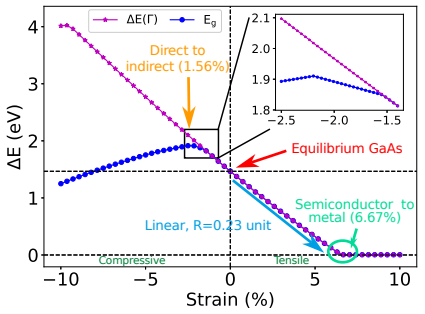
Introduction

Understanding of 'effect of strain' on the electronic properties of III-V semiconductors, widely goes by the name 'strain engineering'; still remains worthy of further exploration, unfolding new possibilities everyday. One of such electronic properties that makes the so-called backbone of optical properties for semiconductors is 'bandgap'. Although a lot of past efforts have been given on the understanding of how the bandgap of III-V semiconductor materials get affected by the strain, those analyses were mostly under hard constraints, such as relatively small strain region only and so on. A complete systematic analysis still remains missing. Further, due to the tremendous increase in 'complexity', all previous analyses were mostly limited to the binary systems. Our goal is to provide a systematic approach for analyzing such phenomenon and develop a relatively cost effective strategy for the extension towards higher order systems, using the tool of computational method, modern *ab-initio* density functional theory (DFT).

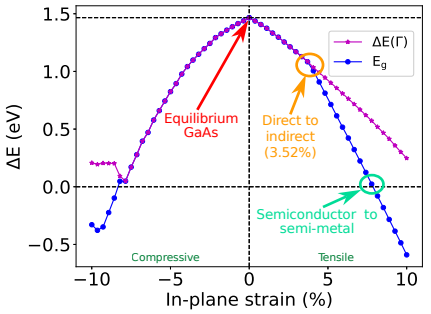
Binary system

- $\Delta E(\Gamma)$ ≡ Energy difference between CB and VB at Γ-point
- E_g ≡ Energy difference between CBM and VBM ≡ Bandgap

- **Direct to indirect transition (DIT) in GaAs:**

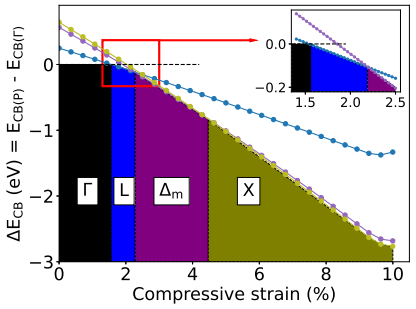


Isotropic strain



Biaxial strain

- **Transitions in GaAs:**



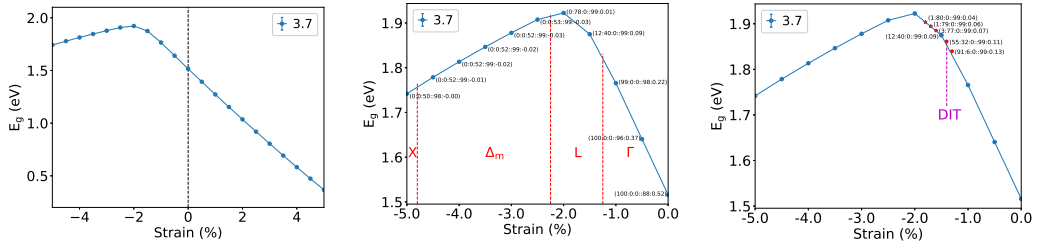
- **Transitions summary:**

System	Transition	Transition (T2)	Transition (T3)
Si	IDT	$\Delta_m \to L \to \Gamma$	×
GaP	IDT	$\Delta_m \to L \to \Gamma$	×
GaAs	DIT	$\Gamma \to L \to \Delta_m \to X$	$\Gamma \to \Delta_m$
GaSb	DIT	$\Gamma \to L \to \Delta_m$	$\Gamma \to \Delta_m$
InP	DIT	$\Gamma \to X$	$\Gamma \to \Delta_m$
InAs	DIT	$\Gamma \to X$	×
InSb	DIT	$\Gamma \to L \to \Delta_m$	×

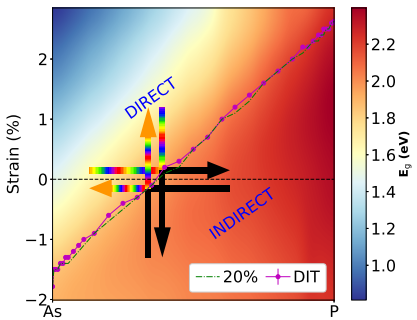
T1 (%) : Semiconductor to metal transition under isotropic tensile strain
T2 (%) : Direct to indirect (DIT) or indirect to direct (IDT) transition under isotropic strain.
T3 (%) : DIT or IDT transition under bi-axial strain

Ternary system

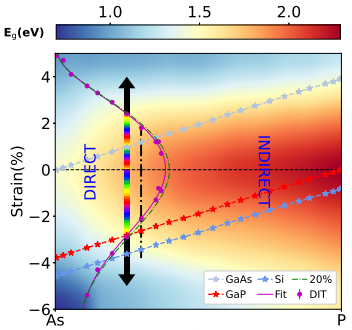
- **Recipe:** CB Bloch weight (Γ:L:X::Δ_m:ΔE_f=(E_Δ-E_Γ)); $GaAs_{0.963}P_{0.037}$



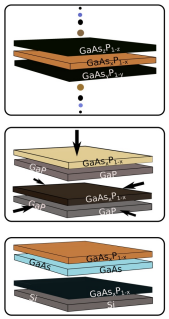
- **Bandgap phase diagram:** GaAsP



Isotropic strain



Biaxial strain



Summary:

1. Depending on the nature and the strength of applied strain the material behavior can change substantially; such as, the otherwise direct bandgap semiconductor can transform to an indirect bandgap semiconductor or vice versa.
2. Develop a relatively simple recipe for the DIT analysis in ternary system keeping the computational cost at its minimum, ultimately enabling us to construct the so-called 'bandgap phase diagram'.

Computational details

Periodic DFT using VASP-5.4.4:
Optimization : PBE-D3(BJ), PAW basis set (450 ev),
Convergence: 10^{-6} eV energy, 10^{-2} eV/A force
Electronic prop.: m-BJ, PAW basis set (350 ev), spin-orbit coupling
Convergence: 10^{-4} eV energy, 10^{-2} eV/A force
Primitive cell : 11x11x11 Γ centered k-mesh.
Super cell : 6x6x6, 10 SQS [3], Γ-only, band unfolding [2, 4]

Remarks

This new way of mapping the effect of strain will significantly improve the future development in terms of strategic choice of certain applications-oriented most suited material systems or vice versa.

Outlook

Extension to the higher order systems. Map other transition regions.

Acknowledgements

This work was supported by German Research Foundation (DFG) within the framework of GRK 1782. Computational resources were provided by Goethe-HLR Frankfurt, ZIH Dresden and HLR Stuttgart.

References

[1] V. Popescu and A. Zunger, Phys. Rev. B **85**, 085201 (2012)
[2] O. Rubel et al., Phys. Rev. B **90**, 115202 (2014)
[3] A. Van De Walle et al., Calphad **42**, 13 (2013)
[4] P. V. C. Medeiros et al., Phys. Rev. B **91**, 041116 (2015)