Strain-induced bandgap transition in III-V semiconductors

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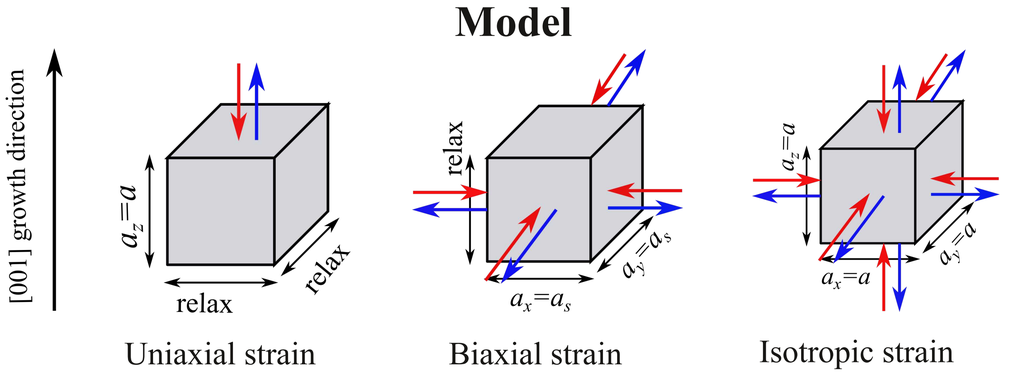
Introduction

The modification of bandgaps in III-V semiconductors is of strong interest for optoelectronic applications. Varying the relative composition is one of the major strategies to tailor the bandgap in compound semiconductors. Strain can be used further to fine-tune. In combination, they can be used to customize the bandgaps over a wide range of values and induce the transition in the nature of bandgaps. Here, we establish a predictive *ab initio* approach based on density functional theory (DFT) to analyze the mutual correlation of composition, strain, and the bandgap of material in multinary III-V semiconductors.

Model

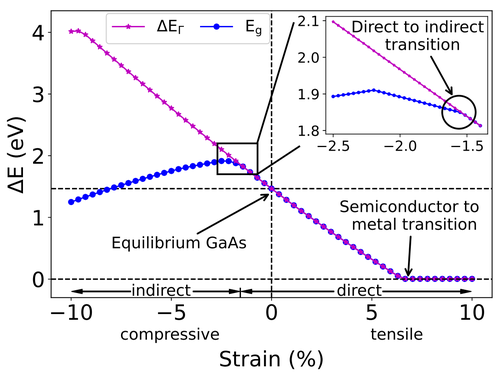


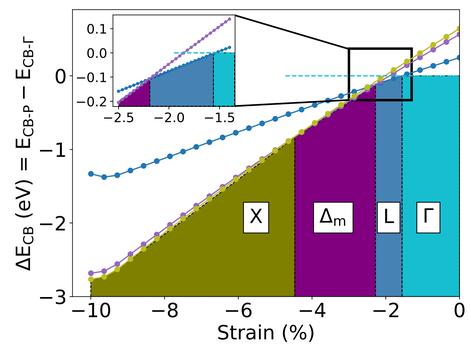
- Compressive strain (–)
- Tensile strain (+)

- Zincblende structure
- $a_s \equiv$ Substrate lattice parameter

Binary system

• Strain-bandgap relationship in GaAs under isotropic strain

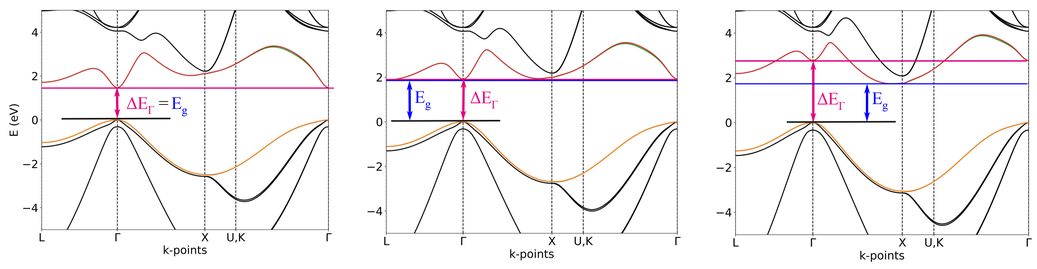




- P = Γ, L, Δ_m, and X point

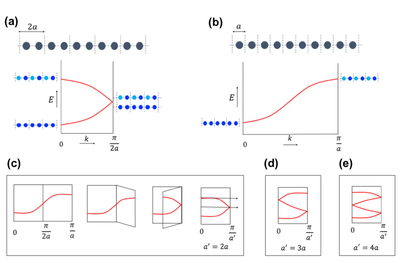
- Valence band maxima stays at the Γ point throughout

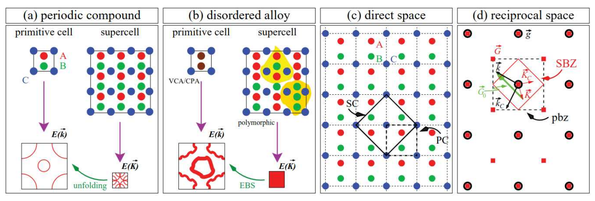
• Evolution of GaAs band structure under compressive strain



Strain = 0.0 % Strain = -1.8 % Strain = -5.0 %

Band folding [1, 2]





- $|\mathbf{K}\ m\rangle = \sum_i^{N_k} \sum_n F(\mathbf{k}_i, n; \mathbf{K}, m)\ |\mathbf{k}_i\ n\rangle$
- $P_{\mathbf{K}\,m}(\mathbf{k}_i) = \sum_n |\langle \mathbf{K}\ m \mid \mathbf{k}_i\ n\rangle|^2 \Rightarrow \sum_{\mathbf{g}} |C_{\mathbf{K}m}(\mathbf{g} + \mathbf{G}_i)|^2$

Ternary system

• Challenge

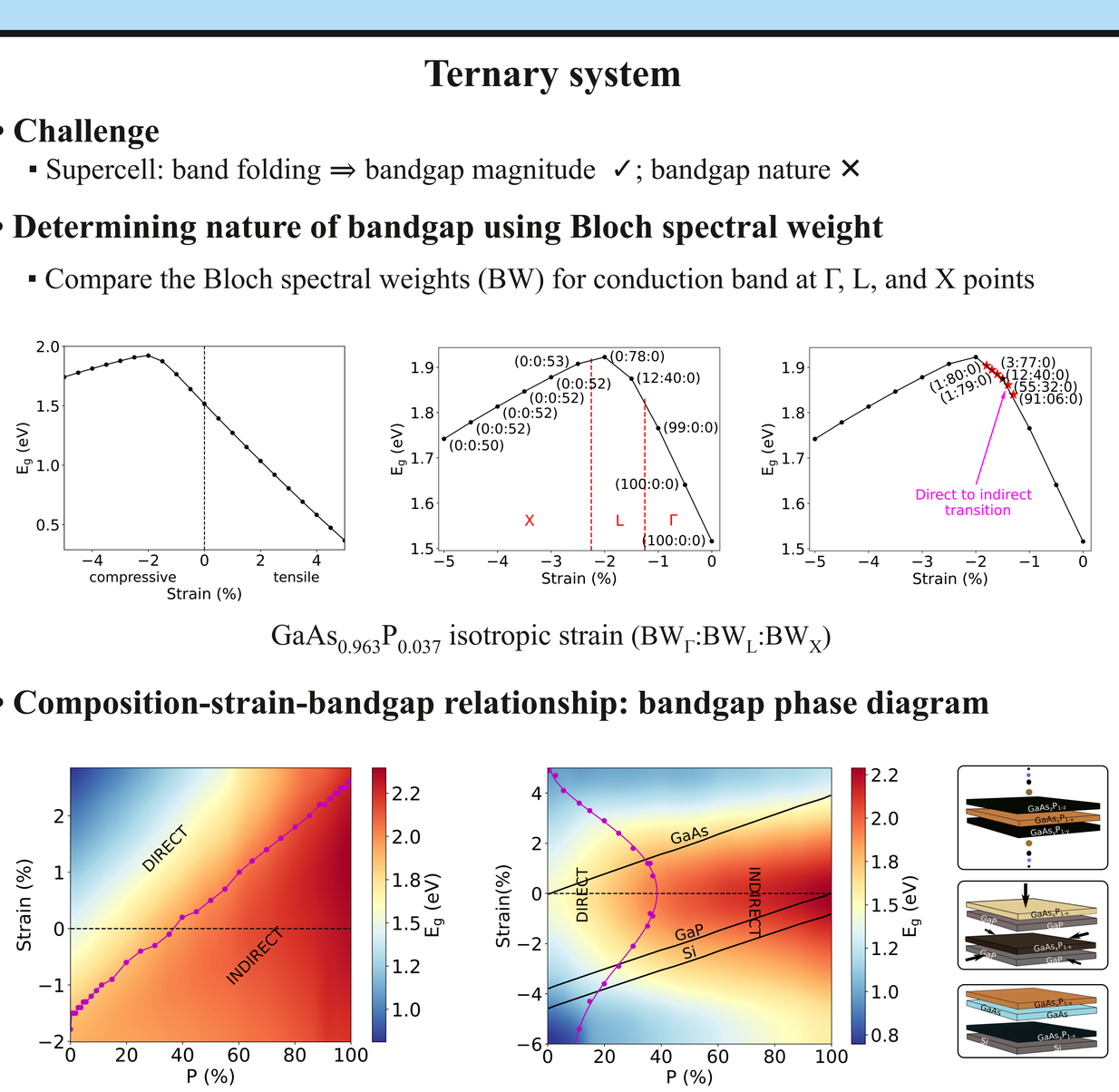
- Supercell: band folding ⇒ bandgap magnitude ✓; bandgap nature ✕

• Determining nature of bandgap using Bloch spectral weight

- Compare the Bloch spectral weights (BW) for conduction band at Γ, L, and X points

$GaAs_{0.963}P_{0.037}$ isotropic strain (BW_Γ:BW_L:BW_X)

• Composition-strain-bandgap relationship: bandgap phase diagram



GaAsP: Isotropic strain Biaxial strain

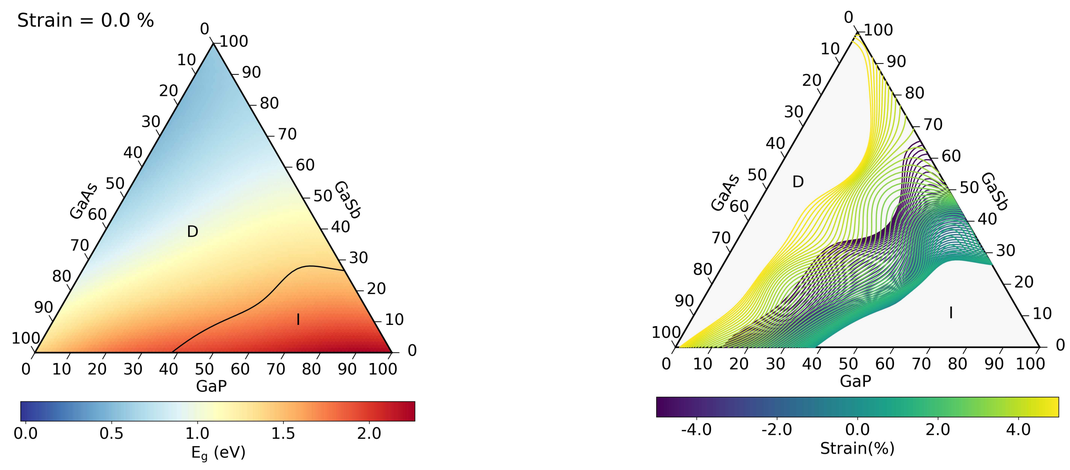
Quaternary system

• Challenge

- Large composition-strain space ⇒ sampling is not efficient with DFT calculations only

• Combining DFT with machine learning

- Model : support vector machine (radial basis function kernel)
- Training set : 3892 DFT data
- Features : composition, strain
- Bandgap magnitude : r2_score = 0.99
- Bandgap nature : accuracy = 0.95



GaAsPSb biaxial strain bandgap phase diagram

Computational details

- Periodic DFT : VASP-5.4.4, PAW basis set
- Geometry opt. : PBE-D3(BJ), 550 eV
- Electronic prop. : TB09, 450 eV, SOC
- Convergence : 10^{-6} eV energy, 10^{-2} eV/Å force
- Primitive cell : 11 × 11 × 11 Γ-centered k-mesh
- Supercell : 6 × 6 × 6, SQS [3], Γ-only
- Bloch weight : band unfolding [4]
- ML model : SVM(rbf)

Summary

- Bandgap nature in multinary system using Bloch spectral weight
- Efficient sampling in multinary system using machine learning
- Composition-strain-bandgap map: bandgap phase diagram [5]
- Direct-indirect transition in the bandgap nature under strain

Outlook

- $A_xB_{1-x}C_yD_{1-y}$, $AB_xC_yD_zE_{1-x-y-z}$, WZ structure, II-VI systems

Acknowledgements

- HRZ Marburg, HLR Frankfurt, ZIH Dresden, HLR Stuttgart

References

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[5] https://bmondal94.github.io/Bandgap-Phase-Diagram, 2022

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