Strain-induced bandgap transition in III-V semiconductors

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Semiconductor compounds attract a great amount of attention both in science and technology due to their immense application range in areas such as optoelectronics or integrated circuits (IC). In the interest of a deep and thorough understanding of the effect of strain on the electronic properties of III-V semiconductor materials, we have presented a systematic analysis of 'strain effect on bandgap' from modern ab-initio point of view. Although a lot of effort has been made to understand how the bandgap of III-V semiconductor materials is affected by strain, no complete picture is available yet. Due to the tremendous increase in complexity, those investigations were mostly limited to binary systems, and very little has been explored for higher-order systems. Here, using the idea of Bloch spectral weight [1, 2, 3], we have developed a systematic strategy for the analysis of composition-strain-bandgap relationship in ternary systems. We have shown that depending on the nature and strength of applied strain in the system the material behavior can change substantially. Namely, a direct bandgap semiconductor can transform to an indirect bandgap semiconductor and vice versa. Furthermore, the bandgap can be tuned over a very wide range. This ultimately enables us to construct the 'bandgap phase diagram' [4] by mapping the different direct-indirect transition (DIT) points with composition and strain. strain and/or composition. Using the advanced tools of machine learning, we have further developed a comparatively cost-effective approach to extend the scope in higher-order systems. In combination with the thermodynamic phase diagram, we have shown that the bandgap phase diagram, this new way of mapping the effect of strain in III-V semiconductor materials can significantly improve the future development in terms of strategic choice of certain application-oriented most suited material systems or vice versa.

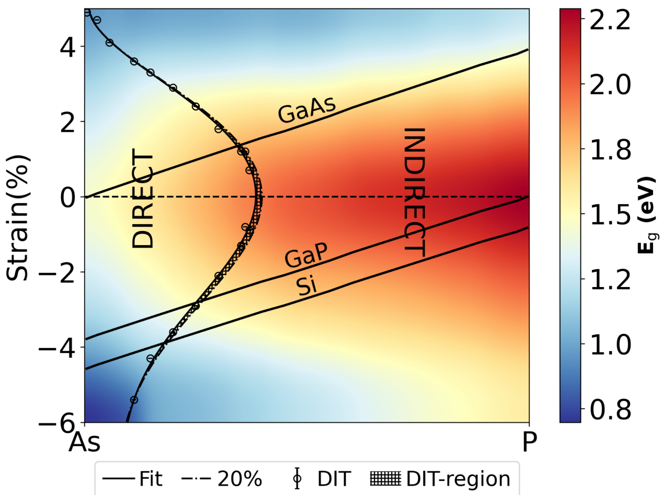

Figure: GaAsP bandgap phase diagram under bi-axial strain. 'DIRECT' and 'INDIRECT' indicate the region of compositions having bandgap direct and indirect in nature, respectively. The colorbar shows the bandgap magnitude (E_g). The DIT-region is the uncertainty in the determination of bandgap nature. The 20% line corresponds to the cutoff of 20% Bloch weight is considered as the minimum criteria in defining a state. The DIT points are fitted with a polynomial of order 5. The GaAs, GaP, and Si lines correspond to the substrate strain line under the 'epitaxial growth' model.

References:
[1] P. R. C. Kent, A. Zunger, Phys. Rev. B 2001, 64, 115208.
[2] V. Popescu, A. Zunger, Phys. Rev. Lett. 2010, 104, 1.
[3] O. Rubel, A. Bokhanchuk, S. J. Ahmed, E. Assmann, Phys. Rev. B 2014, 90, 115202.
[4] https://bmondal94.github.io/Bandgap-Phase-Diagram/