

Strain-induced bandgap transition in III-V semiconductors

Thank you.

Ok, So to start with; the particular system of **our interest**, is the III-V semiconductor family. [FORWARD] And the reason, I think we all here are quite familiar with, is their diverse applications in our everyday life: extending from our daily household LED to modern advanced technologies such as solar hydrogen production. And that's saying, all of these examples here poses a common interest; and that's their optical activity. [FORWARD]

And **one of the fundamental property** that dictates the optical characteristic of an optically active material is the bandgap: both in terms of it's the magnitude and it's the nature, whether it is direct or indirect in nature. [FORWARD]

Now,

one of the reason, the III-V semiconductor family gained so much success in this field of optics; is the possibility to achieve the materials of variable composition, so called ‘compositional engineering’; enabling the ability to achieve immense versatility in bandgaps and thus, the device applications. **[FORWARD]**

As an alternative, another approach has also been adapted in this respect, is the strain engineering, where by straining the system specifically one can tune the electronic properties. **[FORWARD]**

They can appear together as well. For e.g. in ‘epitaxy’. And there, the specific electronic properties of the active layer are dictated by not only the composition of the layer material but the inherent strain from the hetero-structure also play crucial role. **[FORWARD]**

And this builds the stage for our aim. Our goal is to explore and understand this correlation of composition, strain and the bandgap of the materials; **[FORWARD]** using the ab-initio computational approach, density functional theory. **[FORWARD]**

Let's start with the simplest III-V semiconductor family; the 'binary systems'. [FORWARD]

As an example case I will show you today is GaAs. In this case, we don't have anything to vary in composition. So, we only have strain-bandgap relation.

And, here is such a strain-bandgap map looks like for GaAs under isotropic strain. The positive and negative strains correspond to the tensile and compressive strains, respectively. [FORWARD]

Starting from GaAs at the equilibrium configuration, under compressive strain the bandgap initially increases in magnitude, until at about 2% strain when the trend change its direction, the bandgap starts to decrease. Under tensile strain however, the bandgap continuously decreased until at about ~6% strain the bandgap vanishes.

Now this is about the magnitude of bandgap. Recall we also need to map the nature of bandgap.[FORWARD]

For that, we compared the magnitude of bandgap with the CB and VB energy difference at the Gamma point. [FORWARD] If they overlap that would be the bandgap of direct nature and if they deviate from each other **indicate** indirect bandgap. Further, [FORWARD] one can also look at the so-called evolution of bandstructure under strain. [FORWARD] This tells under tensile strain, the bandgap remained direct throughout and decreases in its magnitude only. [FORWARD] For compressive strain, however, the direct bandgap GaAs initially increases in magnitude until at about 1.5% of strain when the CBM at the Gamma point transit to the L-point, and ultimately to the X-point; leads to the transition in the nature of bandgap: from direct to indirect bandgap transition. This confirms the previous as well. [FORWARD]

Take home msg, Straining the system not only change the bandgap in terms of its magnitude but it also affect the nature of bandgap itself. Depending on the nature and strength of applied strain in the system a direct bandgap semiconductor can transform to an indirect bandgap semiconductor.

And we now have a compact way to map this complete strain-bandgap relationship in binary III-V semiconductor materials. **[FORWARD]**

Let's extend the analysis to the next higher order ternary systems. [\[FORWARD\]](#)

In this case, the compound of our choice today is GaAsP. In comparison to the binary systems, now addition of a 2nd component introduces the concept of composition here. So now we have to map the bandgap w.r.t both strain and composition.

Seems straightforward except one slight problem.

Unlike the binary systems where we could use simple primitive cell for the analysis but now to ensure the ideal admixing among all the components we have to use supercell. Now, the use of this supercell results a well known phenomena, something called 'band-folding'. Due to this 'band-folding' although it is straight forward to get the information about the magnitude of bandgap, but not so for the nature of bandgap. And this poses our 1st major scientific challenge: how to determine the nature of bandgaps here?

Fortunately, there has already been an idea in this field of band folding problem for quite a long time, known as 'Effective band structure' concept; where the core idea is to define the bands in terms of something called 'Bloch spectral weight' or short 'Bloch weight'; an artificial way of band unfolding.

And this idea of 'Bloch weight' ultimately enabled us to determine the nature of bandgaps and consequently, to map the composition-strain-bandgap relationship in ternary systems. [\[FORWARD\]](#)

For example this is such a map how it looks like for GaAsP under isotropic strain.

You have the 100% As here and 100% P here. This is your composition axis now. You have the strain here. The colors are the magnitude of bandgaps.

[FORWARD] And then, if you map the nature of the bandgaps as well, you can construct such a separation line that separates the nature of bandgaps of different kinds. Anything in this region will have bandgap direct in nature and anything in this region will be indirect bandgap. This so-called 'direct-indirect' transition line as if separates the band gaps into 2 phases.

These final pictures what we named as 'bandgap phase diagram'. **This can guide you to spot the most suitable choice depending on your need.** [FORWARD]

You want to create an optical device with different optical properties. Pick a particular composition of your choice and then by appropriately straining the system you can make it either direct or indirect in nature.

[FORWARD] At a constant strain, by changing the composition of your layer you can make it direct or indirect. **And you can know this appriori what to do.** [FORWARD]

You can do the same for other kind of strain as well. For example this is how the similar picture looks like for Biaxial strain, GaAsP. This magenta curve again is the ‘direct-indirect transition’ line that separates the two region.

What special about this biaxial strain is that, we can model the ‘epitaxy’ in terms of this type strain. [FORWARD]
If we assume the source of the biaxial strain as the substrate effect from epitaxial growth, then you can add the different substrates here like this. Here I put 3 most commonly use substrates, GaAs, GaP and Si. These lines corresponds to how much strain will be there if you grow let say these compositions on GaAs substrate. You can add other substrates as well. In terms of device application again this picture can help you in different ways. [FORWARD]

For e.g. you can think of a hetero-structure like this. You grow a direct bandgap layer corresponding to this composition with this bandgap on GaAs as substrate and sandwiched it in between two same or different indirect bandgap layer.

[FORWARD] Or, you grow this composition on GaP substrate and then apply small perpendicular pressure from top equivalent to applying tensile strain, then it become direct, and other way around if you apply side-wise pressure mimicking the compressive strain then you can make the epitaxial layer an indirect bandgap. You can make use of this concept for example in pressure sensor.

[FORWARD] You can also make the epitaxial layer either direct or indirect depending on your choice of your substrate, GaAs or Si.

Essentially this way one can choose or determine the best option. Best option in materials combination given an application in mind or vice versa, given a materials combination what can be done with it. **This is completely predictive.**

[FORWARD]

So far, we used the so called direct computational approach to construct the bandgap phase diagram. Starting with a particular composition and strained structure you do quantum chemical calculation such as density functional theory calculation, ultimately get the property that you are interested in, in our case bandgap and its nature. Repeat this strategy at different composition and strain point to construct this whole map. [FORWARD]

Unfortunately, soon we realized for quaternary system increase in one more degrees of freedom almost exponentially increases the compositional space. Just as an hand waiving estimation: from ternary to quaternary such a direct approach would increase the number of DFT calculation needed, to approx 2 order in magnitude. Therefore, it will be a close to impossible approach to take to cover enough of this vast composition-strain space using DFT calculations only. So, we looked for an alternative. [FORWARD]

And ultimately, decided to take the advantage of another uprising modern scientific tool Machine learning. The core idea is to combine our limited expensive DFT capability to the easily extendable machine learning. Train a ML model with the few but enough highly accurate DFT data, learn from the data and ultimately, be able to predict over the full space with relatively inexpensive and minimum effort. [FORWARD]

Using Support Vector Machine in combination with Radial basis function kernel, we established a machine learning model to construct the bandgap phase diagram for quaternary system. This is such a strain snapshot of bandgap phase diagram looks like for Ga(AsPSb) biaxial strain. The D and I correspond to the Direct and Indirect bandgap which are again separated by this separation line. [\[FORWARD\]](#) And then you scan over strains. With only about 4000 DFT calculations training set using our machine learning model we were able to reach an excellent accuracy of ~95-99% in terms of predictions, here. [\[FORWARD\]](#)

So,

to summarize; in the interest of understanding of the effect of strain on the bandgap of multinary III-V semiconductor materials, we have established a recipe for the analysis the composition-strain-bandgap relationship; which ultimately enables us to construct the so-called 'bandgap phase diagram'. I showed you the construction of bandgap phase diagram in Binary, Ternary and then in Quaternary systems, respectively. In the way, we solved two of major scientific challenges: on going from binary to ternary our 1st challenge in terms of band folding using the idea of Bloch spectral weight and then going from ternary to quaternary: establish an efficient alternative to reduce huge the computational cost, using Machine learning.

Hopefully, I was able to convince you the **great benefit and predictive power** of this new mapping in semiconductors. **[FORWARD]**

Just as a final note: for convenience I have presented here only selected choice of the systems as examples. We also did for other systems and details you will find here. [\[FORWARD\]](#)

With this, I am at the end. I would like to thank my supervisor Prof. Ralf Tonner-Zech. Many thanks to all of our collaborative supercomputer centers. And finally, thank you for your attention. [\[FORWARD\]](#)

Speculations