

# Strain effect on III-V semiconductor bandgap

First of all thank you \_\_\_\_\_ for the nice introduction. And good morning and welcome from my side. Let me start by thanking \_\_\_\_\_ who 1<sup>st</sup> suggested me for presenting this work to this audience. And obviously many many thanks to this seminar organization committee for giving me the opportunity to present our research. If I am not mistaken then I am quite aware that all of my audience here are experts in the III-V semiconductor field. But still to make things consistence I would like start with a short introduction. After Si that revolutionized the world in terms of modern electronics, around 1950-60's the discovery of a new family of semiconductor, III-V semiconductor, reshaped the world in terms of modern opto-electronics. [FORWARD]

Thanks to their unique characteristics of tunable electronic properties their diverse application stretched from our daily household LED to [FORWARD] modern LASER, [FORWARD] Solar cell to [FORWARD] optical telecommunication to, [FORWARD] modern Solar hydrogen production technology are only few of them to mention. Since its discovery people are trying to understand the whole field from different perspective, trying to develop new techniques, unfolding new possibilities everyday.

One of such particular area in this field that has gain a lot of success in the past few decades and still doing so, goes by the name 'strain engineering'. [FORWARD]

Strain either by some external means such as by pressure application [FORWARD] or in the form of inherent strain, such as in hetero structure [FORWARD] or some time by means of unavoidable environment effect such as the effect of temperature. For a long time both from experimental and theoretical perspective people are trying to understand how these strain affects the different electronic properties of III-V materials, in the goal of either use them for our good or sometimes to avoid them. [FORWARD]

One of such electronic properties that makes the so called backbone of optical properties of semiconductors is 'bandgap', both in terms of it's magnitude and nature. Although a lot of past effort has been given on understanding of how the bandgap of III-V semiconductor materials get affected by strain, but due to tremendous increase in so called '**complexity**', most of the previous analyses [FORWARD] were limited to small 2-component binary systems. Very little has been explored for higher order system. Our goal is to develop a systematic strategy for such analyses for higher order systems [FORWARD] using the tools of 'computational method', modern ab-initio density functional theory. And today I would like to show you at least the next higher order ternary system.

My story begun with the compound GaAsP, an extremely important and experimentally well studied a ternary system, a promising candidate for LASER. This shows how the bandgap of GaAsP with 3.7%P concentration changes under strain. The positive and negative strain corresponds to the tensile and compressive strain respectively. Apart from other features one of the most important features that attracted our attention at the first place in this figure was this -ve strain part, this deviation from apparent linearity. [FORWARD] And that's because; one of our previous similar analysis in binary systems for e.g. in GaAs this observation of deviation turned out to be due to the transition in the nature of bandgap from direct to indirect in nature. So, the immediate question is, is this also a similar effect happening here or something else? How can we analyze this? [FORWARD] So, lets zoom in to the part that we are interested in. And our goal is to understand the origin of this deviation, whether it is direct-indirect transition or not, and where that lead us to.

But if you recall, as I mentioned few minutes ago, unfortunately, on going from binary to multi-nary system the so called 'complexity' for the necessary analyses increases by huge amount. What I mean by the 'complexity' is this. [FORWARD]

In comparison to the binary systems where we could use simple primitive cell for the analysis but now to ensure the ideal admixing among all the compositions we have to use supercell. Now, alongside tremendously increasing the computational cost, which may be resolvable given the modern huge computational power and resources; as most of you probably well aware of, the use of this supercell results the well known ‘band- folding’ phenomena, and that poses one real scientific challenge. Because, due to this ‘band-folding’ although it is straight forward to get the information about the magnitude of bandgap which is plotted here, but it is extremely difficult, not to say impossible to know the nature of bandgap, which however is the most essential component for the analysis of direct-indirect transition that we are looking for. Fortunately, there is a way out. **[FORWARD]**

There has already an idea well known in this area of ‘band folding problem’ for quite a long time, known as ‘Bloch spectral density’ or equivalently ‘Effective band structure’ concept. Now, I don’t want go into details of the ‘band unfolding’ topic. But just to give you an essence, in short the core idea of ‘band unfolding’ is essentially to quantify how much of an unfolded k-point is contributing to a folded k-point, a weight of an unfolded k-point to a folded k-point, which we will call as the Bloch weight now on. Using this idea of Bloch weight we were able to ‘artificially’ unfold the bandstructure and was able to extract the information about the nature of bandgap. **[FORWARD]**

How it looks like? Let’s take an example case GaAs. This is bandstructure of GaAs in its full glory, bandstructure using primitive cell. Now, imagine you are doing supercell calculation in GaAs. In the supercell bandstructure bands will be folded. Interestingly however, the pattern of folding can be predetermined and that depends on your supercell dimension and k-path. And hence, the folding of the band can be pre-known or in our case can be pre-controlled by choosing the supercell size. And this has an advantage in our case. **[FORWARD]**

Because, from our previous binary analyses we also knew that most important k-points those are responsible for direct to indirect transition to happen are G, L and X points in the conduction band. So, by choosing appropriately the supercell size we could fold these 3 most important k-points to the Gamma-point and do the DFT calculation using only single k-point, Gamma-point. And at the end, the idea is to calculate the Bloch weight corresponding to these 3 k-points in the folded supercell **conduction band only** and compare them. From computational perspective this approach saves a lot of expensive DFT calculations cost with the minimum loss of most important information that we were needed for our analyses. Anyway, **[FORWARD]**

For e.g. in equilibrium GaAs or at strain=0, using this approach you would expect to get 100% Gamma-Bloch weight in the folded CB, because the L and X point will be folded at the higher energy bands. **[FORWARD]**

If you go to a configuration like this then you will get 50:50 contribution at the G and L point **[FORWARD]**

and then if you consider a state like this then you will get maximum X- Bloch weight and 0% G-Bloch weight. And accordingly this way you would be able to determine the position of the CBM and hence the nature the bandgap. Keep in mind that the VBM in the way always remains at the G-point. **[FORWARD]**

Very briefly this is how it would look like in our case of GaAsP. Here, this 3 numbers corresponds to corresponding Bloch weight of G, L and X point for the folded conduction band. Once you do that you immediately see that we started with the maximum G-Bloch weight corresponding to CBM at the G-point and hence the direct bandgap and then with strain the G-Bloch weight decreases and L Bloch weight increases, signs the L-point is coming closer to the G-point and then L-Bloch weight dominates corresponds to the shift of CBM at the L-point and hence the direct to indirect transition in the nature of bandgap. And this continues further, from L to X and so on. **[FORWARD]** In short this way you can categorize the different transition regions. And for the time being if we forget about other transitions and focus only on the direct-indirect transition, in this example

case G to L transition [FORWARD] then you can make this line much more precise by doing some extra calculations near this region. [FORWARD]

And then if you do this for every P composition and collect the DIT point and plot them together you can construct such a diagram. You have the 100% As here and 100% P here. The positive and negative strain corresponds to the tensile and compressive strain, respectively. This magenta dots and the corresponding connecting line is the 'direct-indirect' transition line. [FORWARD]

The most amazing thing about this picture is that it divides the whole region into two. Anything in this region will have bandgap direct in nature and anything in this region will be indirect bandgap. [FORWARD] In fact you can determine with quite a good accuracy at which P concentration 'equilibrium' GaAsP itself will transit from direct to indirect bandgap in nature given by this intersection of 0-strain line with the DIT line. [FORWARD]

To complete the picture we can go one step ahead and add the bandgap magnitudes as well in the background. Now, this is for GaAsP isotropic strain. You can do the same for other kind of strain as well. [FORWARD] For example this how the similar picture looks like for Biaxial strain. This magenta curve again is the 'direct-indirect transition' line that separates the two region. Just as a side note, it turns out this difference in behavior between isotropic and biaxial case you can understand it from simple binary approximated band structure picture.

[FORWARD] Anyway, these final pictures what we named as 'bandgap phase diagram'. Here the DIT lines as if separates the band gaps into 2 phases, direct and indirect and hence, the name. Great. What we can do with it. Well we can use this map as an user guide. In short this picture can guide you to spot the most suitable choice or what is called 'sweet spot' depending on your need. [FORWARD]

For. e.g let say 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] You can probably think of a device where you are only allowed to use a constant amount of strain. Then by changing the composition you can make it direct or indirect. And so on so forth.

[FORWARD] If we assume the source of 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 I believe, GaAs, GaP and Si. These lines corresponds to how much strain will be there if you grow let say these compositions on GaAs substrate. 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 can 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. If you don't want the indirect bandgap layer then you know you are allowed to use compositions only within this region. This figure will give you the information about the restricted regions of possibilities.

[FORWARD] Or, you can think of a device like this composition grown on GaP 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] Or, in some application related circumstance, let say you don't have option or flexibility in composition variation. Then you might think of like this. You take two different substrate side by side, for e.g. Si & GaAs and can make the epitaxial layer either direct or indirect depending of your need.

[FORWARD] As I am going close to my time limit, without going into details which can discuss at the end, let me just point out some comments on uncertainty in this respect. For e.g. when we use multiple random structures for each configuration (composition+strain) then you may get different DIT points for different random structures. For e.g. here in GaAsN these vertical error bars essentially correspond to the standard error in the

measurement of DIT points, average over 10 random structures. [FORWARD] You can also get an uncertainty in the composition direction. Then instead of strict DIT line you can define a DIT-region. This side you can think of pure Direct, that side is so called pure Indirect and in-between you have this uncertainty region of transition comes from uncertainty in the Bloch weights. [FORWARD]

With that I am at the end. So, to summarize, I showed you that depending on the strength and nature of applied strain the system behavior can change substantially, an otherwise direct bandgap semiconductor can transit to an indirect bandgap semiconductor or vice versa. Using the idea of 'Bloch spectral weight' we have developed a systematic strategy for the direct-indirect transition analysis for ternary system ultimately enabling us to construct the so called 'bandgap phase diagram' by mapping the different direct-indirect transition points. As an example case I have shown you the construction of 'bandgap phase diagram' for GaAsP and GaAsN under different strain conditions. We believe that our this new way of mapping the effect of strain in III-V ternary (and higher order material) will significantly improve the future development in terms of strategic choice of certain application oriented most suited material system or vice versa. [FORWARD]

What can we do next? Well, This is just the beginning. [FORWARD]

We have just seen only one of the transition, the direct-indirect transition. But we have also briefly seen how to analyze other transitions in indirect region itself such as L-X and so on. So, one can in-principle analyze the other transitions as well given the needs. [FORWARD]

The bandgap phase diagram we have just seen are 2d. We can add another electronic property such as phonon effect or no. of layer constrain etc. as the 3<sup>rd</sup> dimension. [FORWARD]

You can go beyond ternary, at least given the limitations in visualization we can go up to at least 5 components system. [FORWARD]

What about other material systems, for e.g. II-VI or III-VI systems? [FORWARD]

One can also extend this idea to other areas. For e.g. it turns out using the same idea you can create correlation map between bandgap and split-off energy in the direct bandgap regions. And that you can use for e.g. in Auger recombination type analyses.

Before I finish, let me re-emphasize once again the significance of this work. [FORWARD]

Now, everyone of us here is familiar with this kind of phase diagram. This is the so called compositional phase diagram or thermodynamic phase diagram. As an experimentalist we all here know how important this figures are. [FORWARD] These compositional phase diagram essentially tells if you want to grow a system is it possible to grow it, and if so will it be stable after the growth or so-called phase separate; or whether we need metastable condition. It is firm essential to analyze and understand these compositional phase diagram even before we enter the lab. [FORWARD]

The bandgap phase diagram is another similar phase diagram we are offering. If you think carefully this is one step ahead of compositional phase diagram. Earlier we had only compositional phase diagram which told you if you want to grow something, whether you can or not. [FORWARD] And now our bandgap phase diagram will tell you, whether you want to grow something at the 1st place. You 1st decide what you want to grow and then the concern is whether you can grow or not. However, if you think deeply then you may immediately argue against my claim here. Because, in deep sense, these two questions are intertwined, none of these can be considered superior to other. One complements the other. But my point is that, you can't neglect any one of these. Although, we had compositional phase diagram in the picture for quite a long time. But this other one was missing and now we are giving you the missing piece. We no longer have to rely on our experience or trial and error method but now we have a scientifically consistent systematic way to answer both of these questions.

[FORWARD] Let me finish with this remark, the examples that I showed you as an application of the bandgap phase diagram are just a few of the speculations that we came up with. The broader picture is we are giving you

the state of art map with the zoo of opportunities and rest is up to you to decide what you want and which fits your requirements best. The best analogy we could come with in this regard is this, if you are a sailor you can use our map to choose the best and safe passage. And if you are yourself an explorer then we are giving you the recipe to draw your own map. And rather than thinking about the topic just as the construction of bandgap phase diagram if you think of this as a new general scientific idea, then you don't have to restrict yourself with bandgap only. Given the possibilities, you can also adapt and implement this idea in other context as well. **[FORWARD]**

At the end I would like to thank Prof. Tonner for all of his insightful thoughts and ideas and critical discussions. Thanks to all of my group members for their excellent suggestions in the way. Thanks to GRK for the funding opportunity. **[FORWARD]**

And finally, thank you all for your attention and particularly for giving me this opportunity. We have also designed a fairly detail map of this whole topic and you can find it here (the site at the footnote). That includes our results, details of the calculation procedure if you want to do it yourself and so on. Feel free to contact us if you have any further questions, any new ideas from your side. The details you will find there.

With that I am open for further questions, comments and suggestions. Thank you all once again.