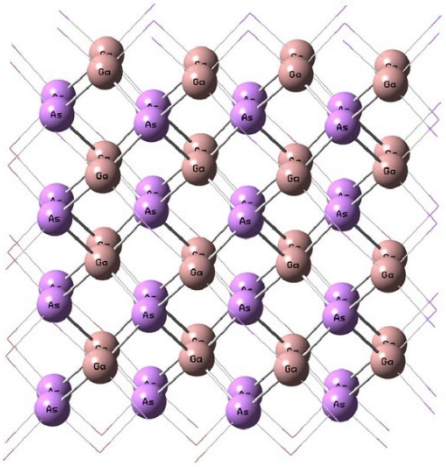
Raiders of the 1.0-1.15 eV bandgap lattice matched material

Welcome back! A couple of weeks have passed but today I am thrilled to publish my third blog post. Despite a long summer break, some activities in the Quantimony ITN took place! During the month of July, I was seconded with four other PhD students to the European Synchrotron Radiation Facility (ESRF) in Grenoble, France. Who wants to find out more about synchrotron radiation experiments should check out the blog of Fernanda. Later in July, all Quantimony students (and some supervisors) came together in Madrid for a Summer School on III-Sb applications with the focus on solar cells. My colleagues work on various topics but during this week, everybody was learning a lot about my personal topic. Of course, I want to keep you updated about my progress as well. That's why within this blog post, you will learn about material engineering and you will be introduced to a super lattice (SL).

Semiconductor Materials

In the last blog post, you were introduced to Multi-Junction-Solar-Cells (MJSCs) and how they can be grown by Molecular-Beam-Epitaxy (MBE). Now, we will be a bit more specific on *why* we need *what* type of material. As a groundwork, two semiconductor material properties need to be understood: the *bandgap* and the *lattice parameter*.

Let's start with the latter: we know that everything on earth is made of atoms. There are different types of atoms which are called elements. If two or more elements are brought together, they do not behave as individuals anymore but form something new. For instance, hydrogen and oxygen form H_2O, water, a substance we are all quite familiar with. When dealing with semiconductors, we are often more interested in their solid, crystalline structure. A crystal is an ordered lattice arrangement of elements. For instance, the elements Gallium (Ga) and Arsenide (As) can form and GaAs lattice (Figure on the right). One property of this lattice is the interatomic distance, in other words, the *lattice parameter.* For MJSCs, we need to grow different materials on top of each other. If the lattice parameter of two stapled materials does not coincide, the material quality suffers, and we obtain bad solar cells. This is like wearing clothes that are too small for you: it doesn´t look great and more important, you might get cold. Therefore, we need a material which can be grown *lattice matched* into the MJSC.



The second semiconductor material property we need to understand is the *bandgap.* A proper explanation would again start with atoms, but I would rather use a picture to explain it: If we as humans want to move around quickly from one town to another, it is beneficial to use the train instead of walking. Let's imagine we are tired, after a long day of work and we are sitting on the railway platform. Then it

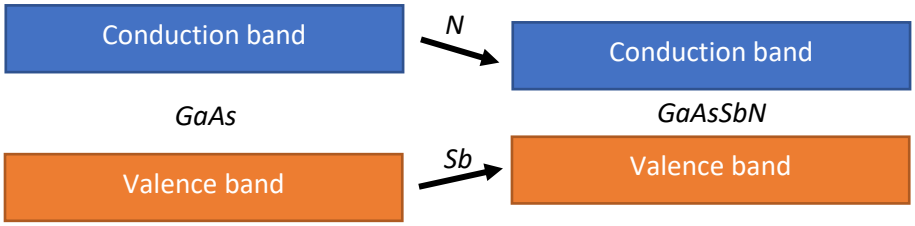
requires some effort, to “hop on the train”: we need to get up and climb the three stairs into the train. If we are tired, we might even need an energy booster, like a Snickers, to get us onto the train. For *electrons* in the semiconductor material, the situation is similar: They tend to rest in their spot (in what is called the *valence band*) and only, upon an energy boost, they hop into the *conduction band.* In the conduction band, they can travel freely through the material as we travel effortless through the country in highspeed trains.

The energy needed, to “hop on” depends on the environment. If we need to climb (hypothetically) 50 stairs to get onto the train, a leaf of salad does not provide enough energy to do so. The same applies for electrons: They need a material-dependent energy, to hop into the *conduction band.* This energy, called the *bandgap,* depends on the material, and is described by units of *electronvolt* (eV). (We could as well use another unit of energy such as the *wavelength, joule* or *calories* in case of the Snickers, but here we will stick to *eV.)*

To grow a very efficient MJSC, it has been shown that a material of 1.0-1.15 eV bandgap is needed. [1, 2] While such a material in general is easy to find, the challenge is to find one that can be grown lattice matched to GaAs or Germanium. It now comes to use what we have learned about the lattice parameter and the bandgap.

Material Engineering

The goal is to grow a material of 1.0-1.15 eV band gap onto GaAs. We could either look for a material with an adequate bandgap and try to modify the lattice parameter, or we start with a material of adequate lattice parameter and modify the bandgap. We choose the latter:
GaAs itself has a bandgap of 1.43 eV at room temperature. The idea is now, to grow an alloy of GaAs, with as smaller bandgap, but similar lattice parameter. We can do so, by growing **antimony (Sb)** and nitrogen (N) into GaAs. Nitrogen has the capacity of reducing the energy level of the conduction band and antimony increases the energy level of the valence band. This is schematically shown in the sketch above. If you want to remain in the train-picture: the Sb is like a lifting ramp on the railway platform (valence band) and the N is like a lowering suspension for the train (conduction band): both ease hopping onto the train.

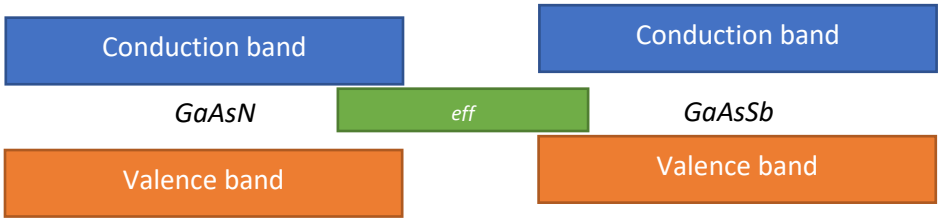


At low concentrations, Sb and N mainly modify the bandgap without altering much the lattice parameter. Therefore, this quaternary alloy fulfils the requirements quite well.

Unfortunately, growing Sb and N together into one alloy, makes suffer the material quality. This means, that the Sb and the N atoms are not distributed homogenously across the material. Rather does this quaternary alloy contain clusters of atoms and many defects, making it a bad material for a solar cell.

Super Lattices

With the problem formulated, you are ready to being presented one solution: a super lattice (SL)! Without going further into detail on the origin of its name, we just look at the main idea:



Instead of growing Sb and N into a quaternary alloy, both are separated spatially into alternating layers of GaAsN and GaAsSb. In this way, good material quality can be assured, and the small **1.0-1.15 eV band gap** is reached "effectively" at the interfaces between the alloys (sketched above).

Conclusion

In this blogpost we have learned that the semiconductor materials of our interest have a characteristic bandgap and a characteristic lattice parameter. We have seen that the bandgap can be modified by growing a many-element alloy, but this reduces the material quality. Last but not least, a spatial separation of the Sb and N atoms into a GaAsSb/GaAsN super lattice has been presented as a "metamaterial" that fulfills all requirements:

- 1.0-1.15 eV bandgap
- Lattice matched to GaAs
- Good material quality

If the last part on the super lattice was too quick: no worries! We will come back to that as the SL is a main part of my PhD. See you soon!

References

1. Kasidit Toprasertpong, Hiromasa Fujii, Tomos Thomas, Markus Führer, Diego Alonso-Álvarez, Daniel J. Farrell, Kentaroh Watanabe, Yoshitaka Okada, Nicholas J. Ekins-Daukes, Masakazu Sugiyama and Yoshiaki Nakano, Progress in photovoltaics 24, 533 (2016).

2. S. R. Kurtz, D. Myers and J. M. Olson, PVSC 875 (1997).