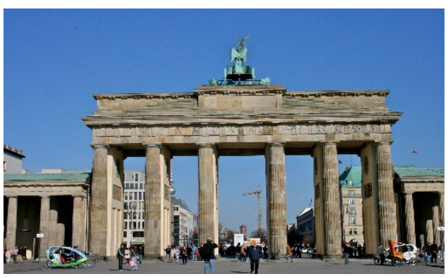
I am back from hibernation!

Welcome back! I am sorry, I know it has been a while ☹ But since my last blog post, I have been anything but inactive. In this post I am telling you about the two Quantimony events that took place: 2nd III Sb Workshop on Structural, electronic and magnetic characterisation and Winter School in III-Sb applications: non-volatile memories – A Modelling Perspective. Furthermore, we will get back to where we stopped last time: The Super Lattice and its application in MJSCs. You will read about my secondment at Fluxim AG in Switzerland and my current temperature dependence study of the current-voltage characteristics of our solar cells.

Quantimony events

Right after uploading my last blog post, I headed off to the Netherlands! At the Eindhoven University of Technology, my colleague Aurelia is working on the *Atomic Scale characterization of III-Sb quantum materials,* which, among others, are our superlattices. What would be a better place to host a workshop in structural, electronic and magnetic characterization? During the three-day event, my fellow PhD students and I got the chance to present our latest progress and engage with invited speakers. My highlights were the presentation of PD Dr. Martin Paul Geller, the lab tour and our visit to ASML – “a relatively obscure Dutch company” (BBC, 2020), I am sure you have heard about!

ASML



The second Quantimony event since my last blog post took place in Berlin. One project partner in our network is Lancaster University, where they developed the ultra-efficient computer memory ULTRARAM™. As many members of our network are somehow related to the ULTRARAM™ research, Berlin University of Technology hosted a *winter school on non-volatile memories – A Modelling Perspective*. The 5-day event included lectures, hands-on sessions, a City-Rallye, and a dinner in the newly opened Humbolt Forum.

SL – a reminder and illustrating simulations

At the end of the last blog post, the GaAsSb/GaAsN superlattice (SL) has been introduced to you as a 1.0 eV bandgap metamaterial that can be grown lattice-matched on GaAs or Germanium in a MJSC. The small **1.0 eV band gap** is reached “effectively”.

The research in my group on these SLs for solar cell applications already goes on for a while. To optimise the material, devices of several layer thicknesses, different Sb and Nitrogen contents and post-growth annealing have been studied. These studies were supported by simulations carried out by a collaborating partner. A simple blog post is surely not the right way to throw these *quantum kinetic calculations based on the non-equilibrium Green’s function formalism* at you, without you probably not having much background knowledge in physics or quantum mechanics. Therefore, I would like to describe the graphic below in other words:

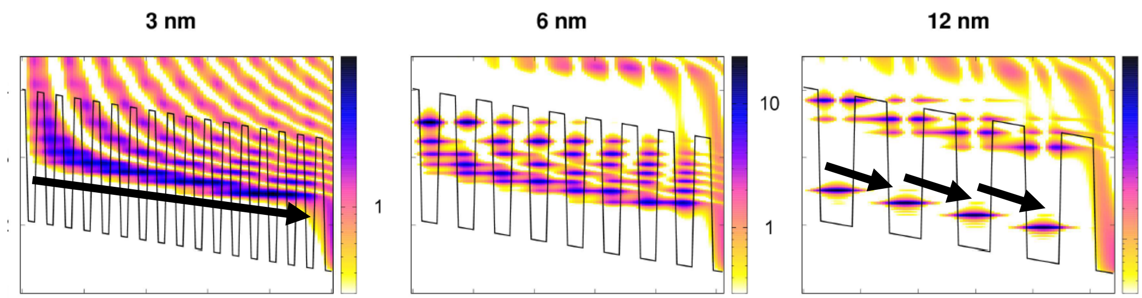


Figure 1 Simulations of SLs of different period thicknesses [1].

What we see are simulations of how electrons are located in the SLs of different period thicknesses. Dark colouring indicates a high probability to find an electron in this spot. Light colouring corresponds to a low probability. We can see that the dark spots are separated in neighbouring wells for thick periods. Though, for thin periods, it looks like there is a continuous band of dark colouring, ranging from the well on the outer left to the well on the outer right. What we want for our electrons, is to travel quickly from the left to the right. And they can travel quickly if they are close to each other, like in the bands of the 3nm SL. They travel more slowly if they are separated, like in the 12nm SL on the right. In this case, they need to hop from one well to the other, like Super Mario needs to jump and run to save the princess. Mario as well would rather choose a flat surface to run after the princess, instead of jumping around in fear of falling. The same goes for the electrons: It is easier to move them from the left to right through the "bands" (3nm SL) than relying on them hopping from the left to right (12nm SL), in fear of losing them and their energy.

Therefore, we prefer SLs of thin periods rather than thick periods.

Secondment at Fluxim AG in Winterthur, Switzerland

The simulations described above are very insightful but heavy to calculate. Most other types of solar cells are typically described by simpler models. Though, those so-called drift-diffusion models do not take the SL structure into account but rather describe effective current fluxes through the device. A company, that provides drift-diffusion-based solar cell modelling software is Fluxim AG in Winterthur, Switzerland.

For the months of January and February 2023, I was seconded to Fluxim to get in touch with the simulation software SETFOS and the optoelectronic characterization system PAIOS. Fluxim's whole product line is shown in the figure below.

Figure 2Product line of Fluxim AG, taken from fluxim.com

If you want to characterize a device electronically, you either apply a current and measure a voltage, or you apply a voltage and measure the current. As easy as that sounds, as varied are the different measurement procedures based on current, voltage, and in the case of solar cells: light
This means, there are many measurement techniques, like transient currents, the response to

modulated light intensity and impedance measurements, just to name a few. All techniques give different insights into how the device works and what happens inside. If you want to understand your device profoundly, it is useful to characterize it in many different ways.
Typically, in research laboratories, measurement stations for the different techniques are set up over the years. The advantage of Fluxim's PAIOS system is, that many techniques are combined in one compact setup, and an extensive characterization is launched with one click.
I analysed many of our devices in the PAIOS setup during my secondment. The results are still under interpretation and I hope to be able to give you an update on that soon.

This brings me to the second product I have worked with SETFOS. To me, the simulation software serves two purposes. On the one hand, it allows to simulate the solar cell structure optically and electronically. In this way, I can optimize my solar cell optically, such that all the sunlight that hits the cell, is absorbed, and not reflected. Furthermore, the cell can be optimized electronically, for example, to reduce the leakage current. The second use for me is to simulate and explain the experiments carried out in the PAIOS setup. For example, I have seen in the transient experiments, that my charge carriers have a certain lifetime before they recombine. I suspect that this lifetime depends on deep traps in my material. Now I use SETFOS, to simulate the experiment for material with deep traps. If my simulation matches the experiment, my hypothesis of deep traps in the material is supported. If the simulation does not reproduce the experiment, I have to look for other mechanisms that might limit the lifetime.

I hope this explanation was not too technical and you got the gist. Otherwise, please reach out!

Current-Voltage Measurements at Low Temperature

I wanted to end this blog post with a small glimpse into what I am currently working on: In my lab, they have set up a solar simulator that provides illumination conditions as if we would measure a solar cell out in the sun. To study transport and recombination in my solar cells, it is useful to study their behaviour as a function of temperature. Now I can do this under realistic illumination, which leads to interesting measurements. But I don't want to overload you with too much information this time, so my IV study as a function of temperature will find space in my next blog post!

Until then, stay tuned and see you soon!

References

1. U. Aeberhard, A. Gonzalo and J. M. Ulloa, Applied physics letters 112, 213904 (2018).