Popular scientific description

What do the chips in your computer, the LED-based lights on your ceiling, and the solar cells on your roof have in common? They are all made out of semiconductor materials. Semiconductors are materials that only conduct current under certain circumstances and offer the possibility to finely tune when there is current, and how many electrons carry it. This is, for example, what allows the transistors (electronic switches) in your computer to turn on and off. In the search for technological advancement, scientists are constantly looking for better, faster and smaller combinations of semiconductors. In this thesis I research a relatively new selection of semiconductors, called polytype semiconductors, for possible applications.

Semiconductors, as the name suggests, only conduct current, under specific circumstances. The reason for this is the physical property called the *energy bands*. Semiconductor materials have bands of possible energy levels electrons can have. One can compare such a band to a box filled with marbles. A marble at the top of the box has more potential energy due to gravity than a marble at the bottom of the box. However it is impossible for the top marble to lose that energy since it is being supported by all the marbles below it. In a similar way electrons in an energy band have different energies due to being "stacked" on top of each other.

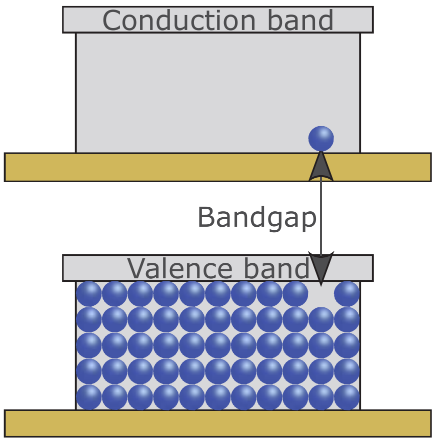

Figure 1: A box completely filled with marbles and a completely empty box. This is similar to energy bands in a semiconductor.

Now imagine two separate marble boxes on a shelf above each other, such as in figure 1. The bottom box is completely filled with marbles while the top box is completely empty. In neither box is it possible for marbles to move in this scenario, since the top box is empty and the bottom box is so tightly packed with marbles that even if you tilt the box they are not able to move. However, if you would raise one marble from the bottom box to the top box, adding potential energy to that one marble, suddenly it would be possible for marbles to move. Not only that one marble in the top box can move, but also the hole in the bottom box can move, because of marbles filling up the space left where one was taken out.

This is similar to what happens to electrons in semiconductors. An electron gets raised from the completely filled *valence band* to the completely empty *conduction band*, leaving behind a hole. For this to happen the electron needs to get enough energy to overcome the so called *bandgap* between the two bands and it is not possible for the electron to exist within the bandgap. Usually the electron gains this energy through heat or light, or by an external voltage. It is possible for an electron to fall back over the bandgap into the hole it left behind and send out light with an energy that corresponds to the bandgap energy. This is the working principle of LED-based lights.

Sometimes it is advantageous to combine different semiconductors with different bandgaps to create so called *heterostructures*. This can be very difficult to do in practice because different materials have different interatomic distances. If you would build the bottom part of a house out of small bricks and the top part of a house out of large bricks, the interface between the bricks will look pretty weird, especially if you attempt to align the large bricks to the small bricks like in figure 2. This is similar to what happens when two materials with different atomic distances are combined: the interface will experience strain because the bricks don't fit. Another problem with combining different materials is that the interface will not be sharp. There can be some mixing of the materials, which gives rise to non-ideal interfaces.

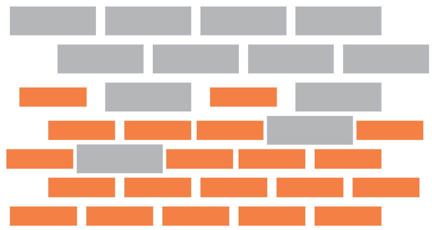

Figure 2: A brick wall using two different sizes brick and intermixing at the interface. This leads to an uneven wall.

I have researched *polytype* semiconductor heterostructures. A material can exist in different crystal structures (different stacking of atoms). Polytype heterostructures are heterostructures made with the same semiconductor material, but different crystal structure. To refer back to the wall example, polytype heterostructures would be like using the same bricks but laying them on top of each other slightly differently, as shown in figure 3. Because of the difference in stacking, the different crystal structures of the same semiconductor material have different bandgaps and energy bands, despite using the same atoms. It is possible to use only a single material to make heterostructures with different bandgaps, while the interfaces are still entirely smooth without strain or mixing.

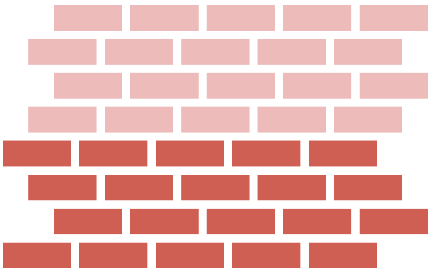

Figure 3: A brick wall where all bricks are the same size but only the stacking order changes. Here the interface is sharp and even.

In my thesis I look at different types of polytype semiconductor heterostructures for different nanoscale applications. Firstly, because nanoscale applications are very small, they have a lot of surface area for very little actual material. Therefore I have looked at the influence of the semiconductor-air interface on the semiconductor properties. I found that this influence is rather large, especially on measurements of the bandgap difference between the two crystal structures. Since all the measurements of polytype heterostructures are done in so called nanowires: small rods of semiconductor material about 100 nm wide (1000 times thinner than a hair), the effect of the semiconductor-air interface should be taken into account whenever bandgap measurements are attempted.

Secondly I looked at the possibility of using polytype heterostructures instead of heterostructures of different materials for high speed electronic components, since the ideal interface could lend itself to even faster semiconductor transistors. In high speed electronics, electrons that carry the current through the semiconductor travel at high speed, often in a very narrow channel of a few nanometers wide. If the walls of this channel are made using material heterostructures, the electrons can bounce against the roughness of the walls, slowing down in the process. In polytype heterostructures that would be less of an issue. I have shown that it is indeed possible to create a polytype heterostructure that could be used as a transistor.

Lastly I looked at really small polytype semiconductor structures called quantum dots. These heterostructures are of the order of 10 nm in each direction, making them 100 billion times smaller in volume than a grain of sand. At this small size the behavior of the electrons is strongly influenced by quantum mechanics. Since the interface of a heterostructure with different materials is not smooth or uniform, the electronic properties of material quantum dots are hard to predict. I have shown that it is possible to create polytype quantum dots with well defined dimensions. I also show that therefore it is possible to predict the electronic properties of these polytype quantum dots before creation. This is crucial for the design of possible applications.