Lattice Matched Interfaces Between Semiconductor Alloys and Metals

Line Jelver, Industrial PhD student, QuantumWise & DTU

Epitaxially matched semiconductor/superconductor interfaces has recently been shown to be a method for creating a material with hard gap induced superconductivity[1]. The two semiconductor alloys $InAs_{1-x}Sb_x$ and $Ga_xIn_{1-x}As$ are combined with a selection of metals to make a semiconductor/metal interface. The interface builder in VNL is used to calculate the strain between the two surfaces of the interface and the alloy parameter x, corresponding to zero strain,is found.

The interface builder in VNL

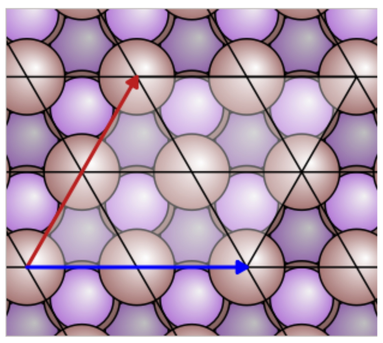

Figure 1a. The interface builder used on InAs(111).

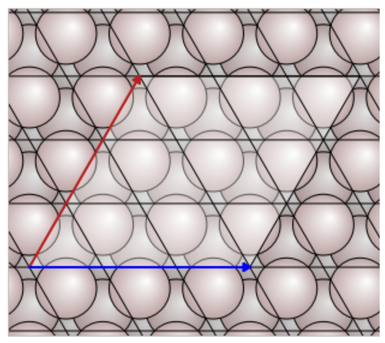

Figure 1b. The interface builder used on Al(111).

The Interface Builder of VNL[2] allows the construction of complex interfaces by automatically matching the 2D unit cells of two different surfaces and compare the strain. Two lattices are matched by finding all possible combinations of unit cells in the first surface and combine those with the best fitting unit cells of the second surface. The strain tensor is calculated for either training the first, the second, or both surfaces. From the tensor, a mean value for the strain can be calculated as:

$$\varepsilon = \frac{1}{2}\sqrt{\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{xx}\varepsilon_{yy} + \varepsilon_{shear}^2} \quad \text{, where} \quad \varepsilon_{shear} = \frac{1}{2}\left(\varepsilon_{xy} + \varepsilon_{yx}\right)$$

Procedure

The two alloys both show linear dependence of the lattice constant with x[3]: $InAs_{1-x}Sb_x$: $6.0583 + 0.4207x$ $Ga_xIn_{1-x}As$: $6.058 - 0.405x$
The alloys have ZB structure and grown nanowires will often show either the $(11\bar{2})$ or (111)surface[4]. These two surfaces are therefore chosen for the investigations. We consider interfaces with with the following metals, using the experimental lattice constants[5]: **Nb, Al, V, Pb, Au, Ag, Cu, Ni, Co, Fe**
For each metal, we consider the surfaces with Miller indices up to 3. The matches with a strain below 2 % and where the total cell size does not exceed 4 alloy unit cells are investigated.

Results

The optimal x-value is found from a linear fit of the cell dilation wrt. x. The results is displayed below, for those matches which have zero strain.

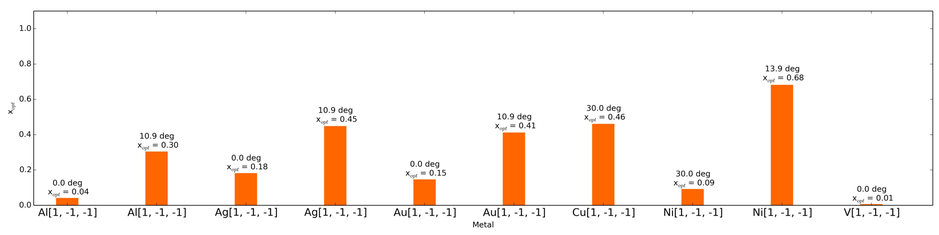

Figure 2a. Optimal x-values for $InAs_{1-x}Sb_x$ $(11\bar{2})$.

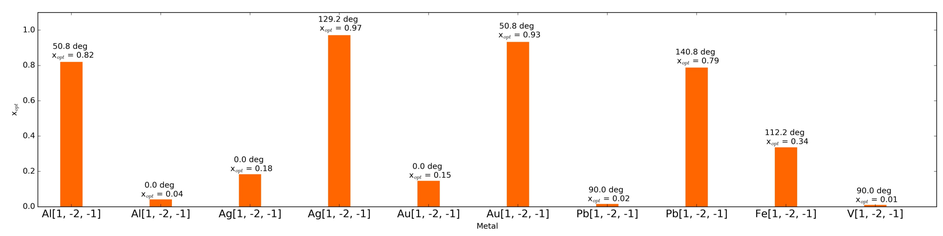

Figure 2b. Optimal x-values for $InAs_{1-x}Sb_x$ (11)B.

Results

For each semiconductor/metal match, one can do a more detailed study. This can be used to make a guess on which surface of the metal that will be grown on top of the semiconductor. The below example is for Al on InAsSb. The fat lines represents the experimental data[4] on the match and the shaded areas shows the color of the surface predicted to have the lowest strain.

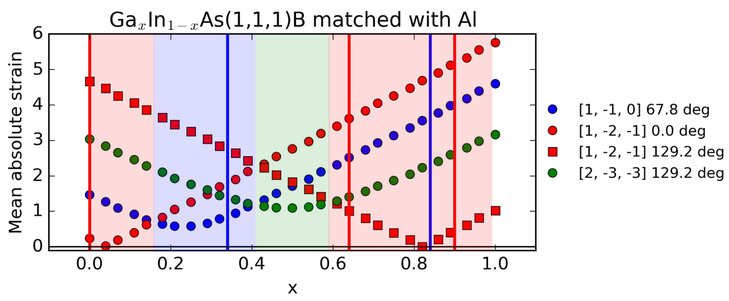

Figure 3a. $InAs_{1-x}Sb_x$ $(11\bar{2})$ matched with Aluminium.

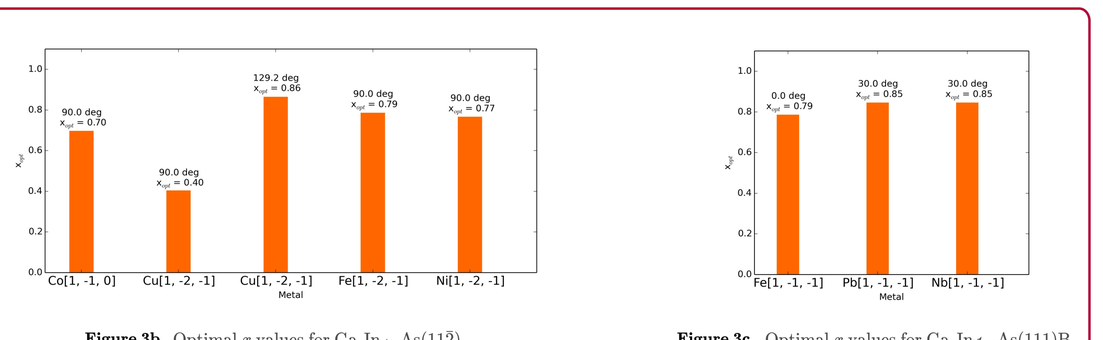

Figure 3b. Optimal x-values for $Ga_xIn_{1-x}As(11\bar{2})$.

Figure 3c. Optimal x-values for $Ga_xIn_{1-x}As(111)B$.

The trend in the experiment is somewhat reproduced but the not all the measurements are predicted. This suggests that the prediction may have to include other effects than the strain between perfect surfaces, e.g. the effect of reconstruction at the surface and grain formation.

References

[1] P. Krogstrup et. al., Nature Materials, Vol 14, 400-406 (2015).
[2] http://docs.quantumwise.com/technicalnotes/interface builder/interface builder.html
[3] http://www.ioffe.ru/SVA/NSM/Semicond/
[4] Unpublished work, T. Kanne et al., Center for Quantum Devices, Copenhagen University.
[5] C. Kittel. Introduction to Solid State Physics. Wiley, 8th edition, 2004.