Master 2 Project: Integration of $Bi_{1-x}Sb_x$ materials on Silicon First principle calculations

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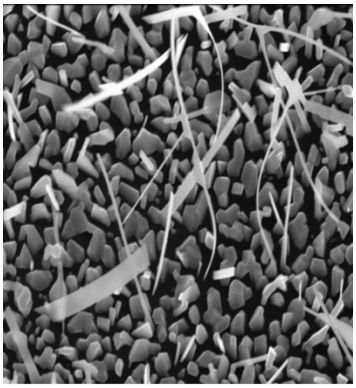
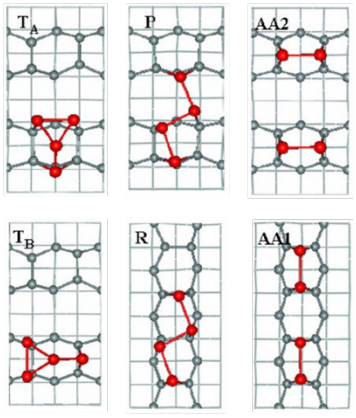
Thermoelectric devices are made from materials that can convert a temperature difference into electricity, making them an ideal too harvest heat loses in any device. The phenomenon is reversible: if electricity is applied to a thermoelectric device, it can produce a temperature difference. Today, thermoelectric devices are used for relatively low-power applications, such as powering small sensors along oil pipelines, backing up batteries on space probes, and cooling minifridges.

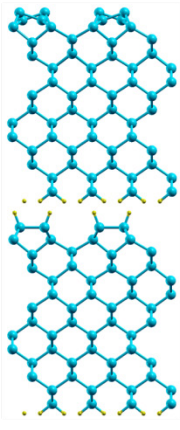
Among thermoelectric materials, bismuth antimonides ($Bi_{1-x}Sb_x$) are used as the n-type legs in many thermoelectric devices below room temperature. The thermoelectric efficiency, given by its figure of merit zT, peaks for compositions x around 10-15%, and belongs to the highest ever reported[1]. Considering a nanowire geometry, the zT coefficient can be improved further by reducing phonon conduction (due to lateral confinement) and keeping the electrical one unchanged.

Here, we propose to study the direct integration of BiSb nanowires on silicon by first principle calculations. This project is a collaboration between MPN and M3. Early results on BiSb integration on Si(001) are already reported (M2 project of Wouter de Jong, see figure 1). We propose to extend this study to Si(110) and Si(111) surfaces as they represent native growth surfaces for BiSb nanowires.



30° Tilted SEM images





	Sb Adsorption Energy (eV)	Bi Adsorption Energy (eV)
TA	4.31	4.74
TB	3.95	4.34
P	4.55	5.08
R	5.00	5.37
AA	9.46	

	Sb Adsorption Energy (eV)	Bi Adsorption Energy (eV)
TA	-0.16	0.26
TB	-0.48	-0.10
P	-1.86	-1.34
R	-1.61	-1.24
AA	0.66	

Figure 1: On left, the direct integration of BiSb nanowires on Si(001).
On Right, the first principle modeling of Sb and Bi incorporation on a Si(001) surface.

References:

[1] Smith, G. E.; Wolfe, R. (1962-03-01). "Thermoelectric Properties of Bismuth-Antimony Alloys". Journal of Applied Physics. 33 (3): 841–846. doi:10.1063/1.1777178. ISSN 0021-8979.