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Understand the formation of the Ni-based silicide/Si interfaces: a DFT study

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Silicides play a significant role in modern device technology [1]. Because of their large use in micro-electronics, a large effort has been done to elaborate and characterize thin silicide/silicon heterostructures [2]. Silicides are alloys formed between a metallic element and a silicon material being deposited due to the intermixing possible by atomic diffusion at interfaces. Even of the use of Ni-based silicides has proven very successful as efficient metallic source/drain junctions, the knowledge on their formation is still far from complete. However, the control of the formation is essential for this application where a thin layer directly integrated on the silicon substrate is desired, which is also the least resistive possible. Even further, the capability to modulate this mixed layer could represent an enormous opportunity for its adaptation to tailored and improved purposes. The formation of a mixed layer during the deposition step has been reported, having its composition a crucial role on the reaction products [2].

Ni silicides sequence formation can be divided into three steps regarding the phase diagram: Ni-rich phases (as $\mathrm{Ni_3Si}$ and $\mathrm{Ni_2Si}$), NiSi, and $\mathrm{NiSi_2}$ phases. From a technological point of view, the target phase is the NiSi one whereas the $\mathrm{NiSi_2}$ phase is not desired as it is more resistive. With the aim to master the final properties of the integrated silicide layer, a detailed knowledge of the process is required.

In this work we study the formation of the multiple interfaces formed during the process of Ni deposition on Si substrates using atomic scale modelling methods based on Density Functional Theory calculations. Starting from deposition, we detail diffusion and reaction mechanisms that form the $\mathrm{Ni_3\,Si}/Si$ interface, then $\mathrm{Ni_2\,Si}/Si$, and finally NiSi/Si interface. Our methodology consists of studying energetically and kinetically favorable atomic diffusions involved in the growth of silicides with a particular focus on mechanisms at interfaces. Eventually, these atomic events will be used to parameterise a Lattice kinetic Monte Carlo code. In addition, this work aims at developing a new Machine Learning interatomic potential adapted to $\mathrm{Ni}_x\mathrm{Si}_y$ alloys.

[1] Murarka, S. P. (1983). Silicides for VLSI Applications Academic Press. New York.
[2] Alberti, A., & La Magna, A. (2013) . Role of the early stages of Ni-Si interaction on the structural properties of the reaction products. Journal of Applied Physics, 114(12), 11_1.

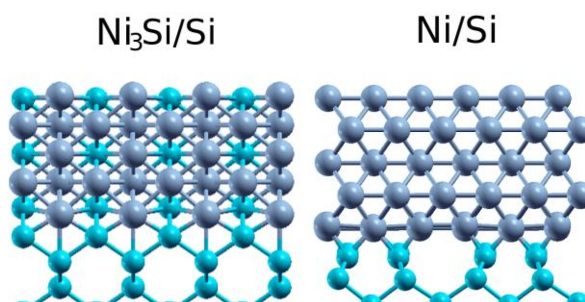

Figure 1 : $\mathrm{Ni_3\,Si}/Si$ and NiSi/Si interfaces.