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Study of Ni silicides formation processes on Si(100) surface using ab-initio calculations

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Silicides are compounds of metals with silicon that play a significant role in modern device technology as efficient metallic source/drain junctions. Particularly, Ni-based alloys are interesting because of their low resistivity, low process temperature, and low Si consumption. The $NiSi$ silicide was demonstrated to be a promising candidate for the fabrication of sub-0.1 micrometer CMOS devices, replacing $TiSi_2$ and $CoSi_2$ alloys. Although the use of Ni-based silicides has proven to be very successful, the knowledge on their formation is still far from complete to obtain a tailored technological process. The formation of the silicide sequence can be divided into three stages based on the phase diagram: Ni-rich phases (Ni_3Si and Ni_2Si), $NiSi$ and $NiSi_2$. From a technological point of view, the target phase is the $NiSi$ one whereas the $NiSi_2$ phase is not desired as it is more resistive. So 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 $NiSi$ silicides formation describing the main steps of the technological process: deposition, interdiffusion and reaction at the interface, using DFT calculations and ART/DFT coupling [1]. All growth events are identified in order to subsequently feed a lattice-kinetic Monte Carlo code. Adsorption, insertion of Ni atoms in the topmost layers of the Silicon substrate in line with the increasing coverage are detailed until the formation of a native alloy formation. Other interfacial reactions are then conducted to investigate the formation of Ni_2Si and $NiSi$ phases. Additional calculations on systems containing interface of interest are done with the aim of developing of an exhaustive and efficient machine learning potential featuring Ni_xSi_y alloys.

[1] Finding reaction pathways and transition states: r-ARTn and d-ARTn as an efficient and versatile alternative to string approaches - Journal of Chemical Theory and Computation16 (2020) 6726-6734 - doi: 10.1021/acs.jctc.0c00541

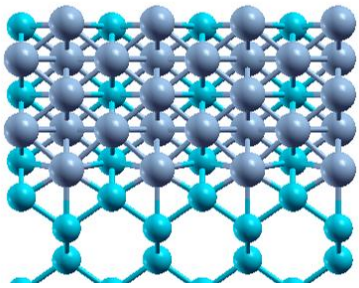

Figure 1 : Ni_3Si/Si interface used in DFT calculations.