T5-I: Hexagonal Si and Ge polytypes for silicon photonics

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The indirect electronic bandgap is the Achille's heel of Silicon, hindering monolithic integration of lasers for Silicon photonics. Metastable hexagonal polytypes of SiGe are very promising to achieve the direct gap within the Si technology. The main approaches to get these hexagonal polytypes and particularly the hexagonal diamond (2H) phase are discussed.
The best quality of 2H Si and Ge has been obtained by exploiting core/shell nanowires [1]: a wurtzite GaAs/P core provides the crystallographic template for the Si/Ge hexagonal shell and together with the lower surface energy of the hexagonal phases allows his epitaxial growth [2]. We will discuss the main problems of this approach from a theoretical perspective, particularly focusing on crystalline defects affecting the hexagonal Si/Ge nanowires (Fig. 1).

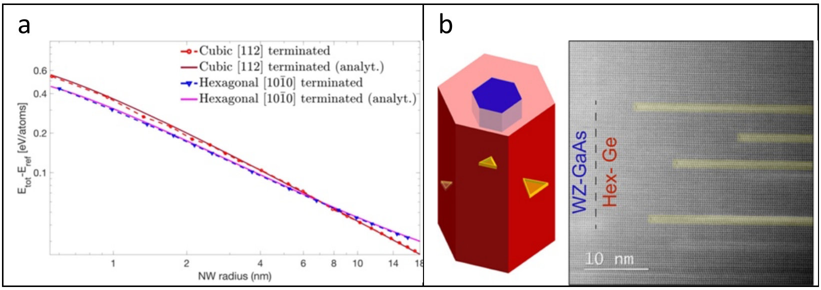

Fig. 1. a) Total energy of 2H and 3C-Si NWs relative to a bulk crystal. b) I3 basal stacking fault in core-shell nanowires.

Then, pressure induced phase transitions in Si and Ge will be presented, focusing on the multiscale modelling of nanoindentation process. In this contest, results obtained with unique methods and novel tools, such as solid-state nudge elastic band (NEB) and machine learning Interatomic potentials, will be also presented [3].

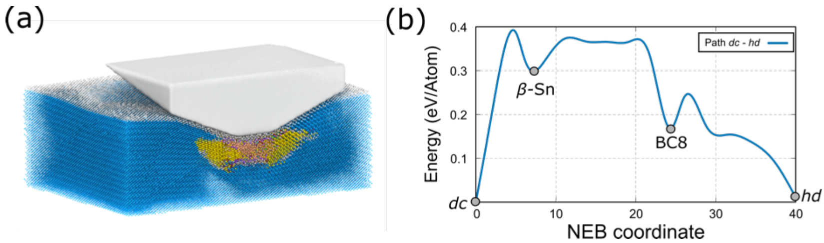

Fig. 2. (a) Schematic view of a MD nanoindentation simulation of silicon. Different colors represent different silicon phases obtained during the nanoindentation. (b) Pressure induced phase transition. NEB calculation of the minimum energy path connecting the diamond cubic (*dc*) to the hexagonal diamond (*hd*) phase of Si. Other phases encountered during the path are highlighted in the plot.

Finally, 2D -hexagonal inclusions in Si and Ge will be discussed. Classically, these would be extended crystalline defects in the cubic phase of Si and Ge, but we will show how these defects could be exploited to form quantum wells with direct gap, potentially very interesting for quantum and optoelectronic applications.

[1] E. Fadaly *et al.*, Nano Lett. **2021**, 21, 8, 3619–3625.
[2] E. Scalise *et al.*, Appl. Surf. Science **2021**, 545, 148948.
[3] G. Ge *et al.*, Acta Materialia, *under revision* (2023)