

# Ab-initio simulation of edge dislocations at a semiconductor interface

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Using first-principles calculations, we have described the mechanism governing the creation of a network of edge dislocations at a high lattice mismatched semiconductor/semiconductor interface. Among all the possible high misfit heterostructures, we focussed on the Si/ $\beta$ -SiC(001) interface without lacking of generality. This system, characterized by a peculiar  $\sim 20\%$  lattice mismatch, can be considered as a template of high lattice mismatched heterostructures, where an ab-initio approach is still affordable. Furthermore, this is a technologically interesting system, because of the outstanding physical properties of  $\beta$ -SiC, that point at a possible candidate for applications in harsh environment devices.

For the studied case, the core dislocation which was found as most stable, and is thus responsible for strain relief in the heterostructure, is pinned at the interface, and occurs at sub-stoichiometric C layers. The presence of these extended defects is responsible for occupied and unoccupied deep level states, laying in the middle of the forbidden gap, which can severely affect the electronic properties of the system.

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