Formation of defects in semiconductors: what contribution from atomistic modeling?

Anne HEMERYCK

[1] *Laboratoire d'analyse et d'architecture des systèmes, CNRS, 31031 Toulouse cédex 4, France*

Corresponding author e-mail address: anne.hemeryck@laas.fr

One of the main drawbacks of the continuous miniaturization of MOS transistors is the increased variability of the device characteristics, in particular the threshold voltage drift. This drift is associated with charge capture and emission phenomena, arising from the presence of defects in the atomic structure of the device that induce electronic states in the band gap of the semiconductor, which can then act as bridges for electrons to thermally cross the band gap, or they become traps for free carriers. These problems stimulate a growing activity around defects in semiconductor materials. In this context, multiscale simulation should allow to anticipate the problems of industrial materials by offering the possibility to review different technological possibilities at lower cost, to help to understand, to optimize and to design new improved materials adapted to specific applications.

In this study, using modeling tools with atomistic granularity, we focus on the atomic mechanisms that cause the presence of these defects in devices, i.e. the mechanisms of defect formation. These defects can be formed either during the manufacturing process, such as ion implantation, or during the use of the components as in radiative environments. In both cases, the ions arriving at high speed destroy the crystal structure of the semiconductor material as they pass through it, leaving behind them defects at the atomic scale. I will describe several approaches ranging from ab initio to industrial technology computer aided design (TCAD) codes and how they can contribute to the understanding of defect formation.
As an example, I will describe how ab initio calculations can help to improve TCAD tools in an industrial context for dopant implantation problems, another example will be the use of molecular dynamics to simulate defects formed under irradiation from the first instants of the cascade. I will also describe the complexity of modeling the growth of material as for example in the case of the growth of silicon oxide.