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Linking design of materials and technological process parameters for tailored integration in Microelectronics field: climbing the scales

A. Hémeryck[1,2], M. Guiltat[1,3], N. Salles[1,2] and N. Richard[4]

[1]CNRS, LAAS, 7 avenue du Colonel Roche, F-31400 Toulouse, France
[2]Univ de Toulouse, LAAS, F-31400 Toulouse, France
[3]Univ de Toulouse, UPS, LAAS, F-31400 Toulouse, France
[4]CEA-DAM-DIF ; Bruyères-le-Châtel ; F-91297 Arpajon Cedex, France

New advanced nanoscale-controlled materials could offer unique functionalities and improve their use in various areas such as the ultrathin films in nanotechnology. Increasing our knowledge and understanding of properties of directly integrated materials at an atomistic level and developing the means of predicting and controlling their structures and functions at the nanometre scale will help to push forward their tailored elaboration. **Understanding how matter organizes at the atomic scale during deposition of ultrathin materials in close relation with elaboration process parameters is the addressed topic.**

It is then necessary to use simulation methods with different length and time scales in order to get a precise description of the physics and chemistry of phenomena but also an overlook on the growth of materials. In our approach, we propose a multilevel approach where modeling / simulation tools are used as a bottom up strategy from atomic scale to simulation platform development linking design and manufacturing. We propose a model based on a kinetic Monte Carlo (KMC) method to simulate growth of directly integrated materials to understand and evaluate the influence of experimental conditions on the nanostructuring and final performances of integrated nanomaterials with the aim to improve their integration into devices. Illustrations on growth of oxide layers under technological processes will be given, notably SiO2 growth through thermal oxidation and CuO growth on Al surface through PVD.

This methodology offers the possibility to access to the exact structure of the material as a function of the manufacturing process and thus to access to the detailed composition, that depends on the conditions in which it was synthesized. We except to propose microscopic elements that could guide the technologist to improve processing and improve the properties of the operating material.