SESSION 5: *New Trends in Surface Science and Coatings*

Contributed Talk – June 17th, 16:35 – 16:50

5-18. A multiscale atomistic method for nanosecond laser annealing simulations

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Heating nanometric portions of a material using nanosecond laser pulses is a very promising route towards future low-temperature processing of 3D sequentially integrated devices. It allows accurate nano-structuring and manipulation of dopants distribution or alloy fraction in the top device layer of a 3D stack without degrading the performance of already fabricated active ones lying beneath it. The main technological challenge is to design the laser annealing (LA) process concurrently with the device design, in order to optimize the topography and the materials' choice in complex 3D nanostructures exhibiting various shapes and phases. To this purpose an atom-by-atom modelling of the phenomena occurring at the nanoscale during LA, such as defect or stress generation and evolution [1], explosive recrystallization [2] and shape deformations, is essential. However most state-of-the-art industrial simulators are based on continuum models and thus lack such atomistic resolution. Here an open-source, parallelized, multi-scale framework to simulate nanosecond LA is presented, based on an algorithm that seamlessly couples a continuum, finite-elements model (FEM) for µm-scale temperature diffusion with a super-lattice Kinetic Monte Carlo (KMC) scheme [3]. After setting up the FEM model with a user-defined CAD geometry, the laser-induced thermal problem is solved until local melting. Thereafter an iterative procedure begins, which for the entire pulse duration, with predefined time resolution: 1) maps the temperature from the FEM mesh to the KMC super-lattice; 2) simulates atom-by-atom the nucleation kinetics and the crystal-orientation dependent solid-liquid interface evolution, accounting for nuclei interactions, defects, stress generation and evolution; 3) updates the solid/liquid state of atoms in the FEM and restarts from 1). Benchmark comparisons against continuum phase-field models and experimental data validate the approach. Applications of the code to study LA of a Si(100) surface will be shown, for two cases of homogeneous and inhomogeneous nucleation, varying laser fluence and pulse duration, revealing how the liquid Si nuclei evolve during laser irradiation, e.g., leading to coalescence for high nuclei densities.

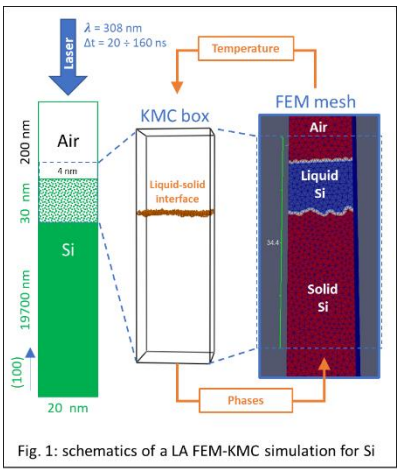

Fig. 1: schematics of a LA FEM-KMC simulation for Si

[1] *L. Dagault et al. Applied Surface Science, 527 (2020) 146752*
[2] *A. Sciuto et al. Proceedings SISPAD 2020, (2020) 71*
[3] *A. La Magna et al. Physica Status Solidi (a), 216, 10 (2019), 1800597*

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