Simulation and Visualization of Thin Film Growth: GPU-based Monte Carlo Approaches

Context

The development of new materials and the improvement of existing ones have been at the core of many advanced applications for decades. Controlling fabrication processes is essential to tailor their shape and properties for targeted applications. Among advanced materials, functional oxides (crystalline transition metal oxides) exhibit a remarkable range of tunable properties (ferroelectricity, transparent conductivity, superconductivity, etc.), which are critical for cutting-edge technologies. In microelectronics, these materials are often fabricated as thin films. However, the relationships between processing conditions and material properties are still largely optimized through empirical approaches, which are both time-consuming and costly. There is therefore a strong need for disruptive methodologies to overcome these limitations and to better understand how deposition parameters influence the evolution of film microstructure (grain size, texture) and properties (defect density, mechanical behavior). This is one of the main challenges addressed by the CINEMA project, which aims in particular to develop efficient GPU-based tools for the simulation and visualization of thin film growth using kinetic Monte Carlo (kMC) methods.

Research topic

Current numerical simulation methods are limited in both time (short simulated durations, hence limited growth) and space (sample sizes too small to compare with experiments). As a result, several important phenomena cannot be properly captured, particularly when studying grain boundaries or polycrystalline growth in thin films. Such simulations typically require extremely high computational cost and memory usage, making them accessible only on supercomputers. Access to these resources is limited and often unsuitable for iterative prototyping phases. Existing methods based on kinetic Monte Carlo (kMC) algorithms are therefore constrained by memory capacity, computation time, and simulation time-step limitations.

Objectives

The goal of this PhD project is to overcome these limitations by addressing both the physical and computational challenges inherent to kMC simulations. The work will focus on three main objectives:

A- Develop a generic out-of-core data management system, capable of handling simulation datasets exceeding main memory limits, while ensuring temporal consistency across billions of atomic events on hybrid CPU/GPU architectures;

B- Enable real-time in situ visualization techniques, providing continuous and interactive access to simulation data, reducing storage requirements and allowing direct visual correlation between growth parameters and film morphology;

C- Accelerate kMC simulations to investigate polycrystalline thin film growth over larger spatial scales and longer time scales. This will allow, for the first time, direct observation of grain boundary formation and evolution, bridging the gap between atomistic modeling and experimental observations.

Candidate profile

The candidate must hold a Master's degree or an engineering degree in the field of computer science.
Strong skills in GPU programming and parallel computing environments are required.
Furthermore, knowledge of or an interest in materials science (physics) is highly desirable.

Contacts

For more information about the project and/or the recruitment process, please contact

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Candidature

Applications must be submitted via the CNRS job portal:

https://emploi.cnrs.fr/Offres/Doctorant/UPR3346-NADMAA-160/Default.aspx?lang=EN