

# CROSS-DIFFUSION SYSTEMS IN MOVING BOUNDARY DOMAINS: DISCRETIZATION AND OPTIMAL CONTROL

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The aim of this talk is to present some recent results about the discretization and optimal control of cross-diffusion systems in moving boundary domains.

One motivation of this work stems from the modelisation, simulation and control of the fabrication process of thin film solar cells. The thin film layer inside of which occur the photovoltaic phenomena accounting for the efficiency of the whole solar cell is done via a Physical Vapor Deposition (PVD) process. More precisely, a substrate wafer is introduced in a hot chamber where the different chemical species composing the film are injected under a gaseous form. Molecules deposit on the substrate surface, so that a thin film layer grows by epitaxy. In addition, the different components diffuse inside the bulk of the film, so that the local volumic fractions of each chemical species evolve through time. The efficiency of the final solar cell crucially depends on the final chemical composition of the film, which is freezed once the wafer is taken out of the chamber. A major challenge consists in optimizing the fluxes of the different atoms injected inside the chamber during the process for the final local volumic fractions in the layer to be as close as possible to target profiles. Two different phenomena have to be taken into account in order to correctly model the evolution of the composition of the thin film: 1) the cross-diffusion phenomena between the various components inside the bulk; 2) the evolution of the surface.

In this talk, we will present two recent results related to the mathematical analysis of this type of systems. The first one concerns the optimal control of the fabrication process: is it possible to identify optimal values of the fluxes of the different chemical species injected in the chamber so that the composition profile of the thin film layer is as close as possible to a prescribed target? The second one concerns a new structure-preserving finite-volume scheme coupling two cross-diffusion systems: one modeling the solid phase, the other modeling the gaseous phase, where the evolution of the domain occupied by each of these phases is determined by the values of the local volumic fractions of the different chemical species close to the interface.

This is a joint work with Clément Cancès, Jean Cauvin-Vila and Claire Chainais-Hillairet.