A Moving-Interface Cross-Diffusion Model for Thin Film Deposition

Clément Cancès[(1)], **Jean Cauvin-Vila**[(2)], **Claire Chainais-Hillairet**[(1)], **and Virginie Ehrlacher**[(2)]

(1) Univ. Lille, CNRS, Inria, UMR 8524 - Laboratoire Paul Painlevé, F-59000 Lille
(2) CERMICS (ENPC) & INRIA, Paris

e-mail: jean.cauvin-vila@enpc.fr

We propose an extension of the one-dimensional model introduced in [1] to describe a vapor deposition process used for the fabrication of thin film layers in the photovoltaic industry. In the process, a wafer is introduced in a hot chamber where chemical elements are injected under gaseous form. As the latter deposit on the substrate, a heterogeneous solid layer grows upon it. We are interested in two essential features of the problem: the evolution of the surface of the film and the diffusion of the various species in both phases, due to high temperature conditions. Our model consists of two cross-diffusion systems coupled by a moving interface through which chemical reactions occur.

More precisely, we consider the moving-boundary domain $\Omega(t) = (0, X(t)) \cup (X(t), 1)$ and n different chemical species represented by their densities of molar concentration $\boldsymbol{c}(t,x) = (c_i(t,x))_{1\le i\le n}$, subject to nonnegativity and volume-filling constraints. The dynamics in the solid (resp. gas) phase is modelled by a size-exclusion (resp. Stefan-Maxwell) cross-diffusion matrix, while the interface reactions are modelled by the Butler-Volmer formulas, given, for some constant reference chemical potentials $\boldsymbol{\mu}^{*,g}, \boldsymbol{\mu}^{*,s}$, by

$$F_i = c_i(X^-)e^{\frac{1}{2}(\mu_i^{*,g}-\mu_i^{*,s})} - c_i(X^+)e^{-\frac{1}{2}(\mu_i^{*,g}-\mu_i^{*,s})}.$$

These formulas appear as flux boundary data at X^-, X^+ of the respective cross-diffusion systems and the model is completed by the interface evolution formula

$$X' = -\sum_{i=1}^{n} F_i.$$

In this communication, I will introduce the model in full detail and present its dissipative structure, using ideas from [2]. I will also characterize the stationary states and discuss long-time asymptotics. Then, I will introduce a finite volume approximation of the system. Although such schemes were previously designed for each respective cross-diffusion system in a fixed domain, the main novelty of our scheme is the treatment of the moving interface. The resulting discrete nonlinear system is shown to admit a solution that preserves the full structure of the continuous system, namely: mass conservation, nonnegativity, volume-filling constraints and decay of the discrete free energy. Numerical simulations illustrate these properties and suggest that the scheme also preserves the long-time asymptotics. A concise presentation of the scheme can be found in [3].

Acknowledgments: The authors acknowledge support from the french ANR project COMODO (ANR-19-CE46-0002) which funds the Ph.D. of Jean Cauvin-Vila.

References

[1] A. Bakhta, V. Ehrlacher, Cross-Diffusion Systems with Non-Zero Flux and Moving Boundary Conditions, *ESAIM:M2AN* **52 (4)** (2018), 1385 – 1415.

[2] A. Glitzky, A. Mielke, A Gradient Structure for Systems Coupling Reaction–Diffusion Effects in Bulk and Interfaces, *ZAMP* **64** (2013), 29–52.

[3] C. Cancès, J. Cauvin-Vila, C. Chainais-Hillairet, V. Ehrlacher, Structure Preserving Finite Volume Approximation of Cross-Diffusion Systems Coupled by a Free Interface, to appear as a proceeding in *FVCA* **10** (2023), preprint available at 10.48550/arXiv.2303.15817.