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Cross-diffusion effects on a morphochemical model for electrodeposition

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ABSTRACT

We analyze the effects of cross-diffusion on pattern formation in a PDE reaction-diffusion system introduced in Bozzini et al. 2013 to describe metal growth in an electrodeposition process. For this morphochemical model - which refers to the physico-chemical problem of coupling of growth morphology and surface chemistry - we have found that negative cross-diffusion in the morphological elements as well as positive cross-diffusion in the surface chemistry produce larger Turing parameter spaces and favor a tendency to stripeness that is not found in the case without cross-diffusion. The impact of cross-diffusion on pattern selection has been also discussed by the means of a stripeness index. Our theoretical findings are validated by an extensive gallery of numerical simulations that allow to better clarify the role of cross-diffusion both on Turing parameter spaces and on pattern selection. Experimental evidence of cross-diffusion in electrodeposition as well as a physico-chemical discussion of the expected impact of cross diffusion-controlled pattern formation in alloy electrodeposition processes complete the study.

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1. Introduction

Reaction-diffusion systems have raised - and continue to raise - a considerable interest because of their intrinsic ability to generate patterns strikingly similar to those found in many chemical, biological and environmental contexts. Such amazing peculiarity is due to the intriguing interplay between diffusion and nonlinear kinetics, which results in the emergence of fascinating self-organized phenomena such as spiral waves, standing waves [1] and Turing patterns [2]. Turing patterns appear in reaction-diffusion systems via Turing instability, a mechanism that can lead to spatial pattern formation when a homogeneous steady state that is stable in the absence of diffusion becomes unstable to an infinitesimal perturbation when diffusion is considered. Moreover for two-variable models, in the traditional biologically-oriented jargon, this kind of instability is described as due to 'long range inhibition and short range activation', i.e. the activator must have a diffusion coefficient smaller than that of the inhibitor [2,3]. Turing diffusion-driven instability is now universally recognized as one of

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the leading mechanisms of spatial self-organization in reaction-diffusion systems and has become the subject of extensive studies in a variety of different applied fields, e.g. chemistry [4,5], population dynamics [6], landscape ecology [7], biology [2,8] and social sciences [9].

However, in multicomponent systems, diffusion cannot be considered as a process involving exclusively individual species in insulation. In fact, according to the specific problem under study, self-diffusion, tracer-diffusion, intra- and inter-diffusion, mutual diffusion, cross-diffusion as well as uphill- diffusion can emerge. For a deeper understanding of these forms of diffusion, we refer to the very detailed discussion developed in [10]. In particular, cross-diffusion refers to the phenomenon in which the flux of a particular species is induced by a gradient of a different one. Cross-diffusion in multi-component systems was theoretically predicted only in 1932 [11] and it was experimentally verified two decades later [12]. Among others [13], recent experiments on the BZ-AOT (Belousov-Zhabotinsky in aerosol OT microemulsion) system [10,14] and on the Oregonator system [15] have revealed that cross-diffusion may be an important element in understanding the many types of patterns found in these systems. Nevertheless, as far as electroplating is concerned, a very limited number of experiments aimed at an insightful understanding of the role of cross-diffusion are available at the time of this writing. It might be worth stressing that the keyword 'cross-diffusion' in the physical metallurgy of metal couples has a different meaning and, from the physico-mathematical point of view it is simple diffusion, possibly with a composition-dependent diffusion coefficient.

The most commonly used constitutive law to model diffusive fluxes within continuum mechanical models is Fick's law, which states that the flux of a chemical component/species goes from regions of high concentration to regions of low concentration, with a magnitude proportional to the concentration gradient [16]. In multicomponent systems, according to the Fickian approach, cross-diffusion processes can be described in the framework of the reaction-diffusion models and are characterized by a Fickian diffusion matrix $\tilde{\mathbf{D}}$ whose off-diagonal elements are both not zero. The diffusion matrix $\tilde{\mathbf{D}}$ is required to satisfy some constraints that derive from the second law of thermodynamics, namely all of its eigenvalues must be real and positive [10,17] but, for thermodynamically stable mixtures, it suffices that $det(\tilde{\mathbf{D}}) > 0$ [18].

Even if the direct proportionality between flux and concentration gradient can provide a reasonable approximation of the diffusion process in a variety of common situations, in other cases this assumption turns out to be too simplistic. An alternative approach to multicomponent diffusion is the Maxwell–Stefan approach by which diffusion takes place in a more complex way than that described by Fick's law. Specifically, to describe diffusion in a multicomponent gaseous mixture, Maxwell [19] and Stefan [20] suggested an explanation of the process based on the binary reciprocal interaction of the gas molecules which accounts for the friction forces that exist between them and introduces diffusivities terms, that can be considered as inverse drag or friction coefficients [10,13], that can be plugged into a system of coupled nonlinear partial differential equations.

From the mathematical point of view, the Maxwell–Stefan equations are far from being fully analyzed. Among the mathematical studies on the topic, relevant to the present paper, we recall: [21] which is focussed on the study of numerical algorithms based on the matrix description of the phenomenon; [22] where a proof is reported on the local-in-time well-posedness of the Maxwell–Stefan multicomponent diffusion system in the isobaric, isothermal case and [23] where a theoretical analysis of the Maxwell–Stefan system is provided in the special case of ternary gaseous mixture and a numerical scheme is also proposed.

In conclusion, it is worth noting that the Maxwell–Stefan approach seems particularly suitable for non-ideal gaseous systems, while Fickian cross-diffusion is the model of choice for the electrodeposition processes we are interested in, as pointed out by the positive experimental evidence proposed in Section 2.2.

There is a huge literature on the mathematical properties of the models related to the Fickian interpretation of the diffusion process. Even within the Fick's approach, the theoretical analysis of the resulting reaction-diffusion systems with cross-diffusion can be a challenging task. Complications can arise from the strong nonlinear coupling and because the diffusion matrix may be neither symmetric nor in general positive definite so that proving even the local existence of solutions is far from being trivial. A well known assumption to prove - at least locally - the existence of solutions is in fact that the diffusion matrix is positive definite, see e.g. [24,25].

A large number of theoretical papers have however specifically analyzed and discussed the effects of cross-diffusion on Turing pattern formation. To mention some, in [10,26], it has been shown that cross-diffusion can promote pattern formation, even through small or negative cross-diffusion coefficients and in [27] cross-diffusion has been considered coupled to linear reaction terms to show that nonlinearity in the source terms is not necessary for pattern formation when cross-diffusion is involved. Madzvamuse et al. in [28], considered the Schnakenberg model and derived conditions for Turing instability driven by both diffusion and cross-diffusion showing that they are a generalization of the classical conditions for Turing instability without cross-diffusion. Moreover, they also showed that - when cross-diffusion is considered - it is no longer necessary that the inhibitor diffuses faster than the activator as well as it is no longer necessary to have an activator-inhibitor mechanism as prerequisite for pattern formation. More recently, in [29], Gambino and coauthors also considered the Schnakenberg model with cross-diffusion and - by using the weakly nonlinear multiple scales analysis - they elucidated the role of cross-diffusion in influencing the occurrence of supercritical or subcritical Turing instability.

In this paper, we follow the Fickian interpretation of the diffusion process and investigate the effects of cross-diffusion on pattern formation and selection in the morphochemical model - called for brevity DIB model from the names of the authors - recently introduced in [30] to describe metal growth in an electrodeposition process and whose spatio-temporal dynamics in the absence of cross-diffusion has been extensively investigated: in [31], conditions for Turing pattern formation

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