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Travelling waves in a reaction-diffusion model for electrodeposition

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Abstract

In this paper we consider an analytical and numerical study of a reaction-diffusion system for describing the formation of transition front waves in some electrodeposition (ECD) experiments. Towards this aim, a model accounting for the coupling between morphology and composition of one chemical species adsorbed at the surface of the growing cathode is addressed. Through a phase-space analysis we prove the existence of travelling waves, moving with specific wave speed. The numerical approximation of the PDE system is performed by the Method of Lines (MOL) based on high order space semi-discretization by means of the Extended Central Difference Formulae (D2ECDF) introduced in [1]. First of all, to show the advantage of the proposed schemes, we solve the well-known Fisher scalar equation, focusing on the accurate approximation of the wave profile and of its speed. Hence, we provide numerical simulations for the electrochemical reaction-diffusion system and we show that the results obtained are qualitatively in good agreement with experiments for the electrodeposition of Au–Cu alloys. © 2010 IMACS. Published by Elsevier B.V. All rights reserved.

Keywords: High order finite difference schemes; Method of Lines; Travelling waves; Fisher equation; Electrochemical modeling

1. Introduction and the model

Electrodeposition of Au–Cu alloys from cyanocomplex baths containing free cyanide has been shown to exhibit electrokinetic instabilities that can lead to compositional heterogeneity in the electrodeposit bulk [4]. Such instabilities derive from a hysteretic current–voltage characteristic related to the buildup of CN^- concentration in the catholyte and attending variations the Cu(I)- cyanocomplex nobility [6]. The technological drawbacks deriving from such instabilities can be efficiently removed by changing the solution chemistry: (i) removing the free- CN^- and (ii) changing the Cu(I)-cyanocomplex for a Cu(II)-EDTA compound [5]. Notwithstanding the technological improvement, a rich dynamic scenario is still attached to the presence of adsorbed CN^- at the growing metal interface [9].

In this paper we consider a general model coupling the surface morphology and CN^- concentration, in order to rationalise the formation of the morphological patterns sometimes developing in electrodeposition (ECD). Some dynamic details will be discussed with model parameter values typically corresponding to the more industrially widespread free- CN^- solutions. This phenomenon is a special case, original within the realm of metal electrochemistry, of a more general, well-known type of chemical and electrochemical dynamics (electrocatalysis [18], corrosion of Cu [15], Fe-group metals [18] and Ag [8]).

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