Pattern Formation in Catalytic Processes: Phase–Field Model

M.N. Kuperman[1], A.S. Mikhailov[2], and H.S. Wio[1]

[1] Centro Atómico Bariloche (C.N.E.A.) and Instituto Balseiro (U.N.C.) 8400 - San Carlos de Bariloche, Rio Negro, Argentina
[2] Fritz-Haber Institut, M.P.G., Faradayweg 6, Berlin, Germany.

We present a first step towards the modeling of adsorption and desorption of CO in empty sites during its catalytic oxidation on a Pt monocrystalline surface ($2\ CO + O_2 \rightarrow 2\ CO_2$). After a diffusion process on the Pt surface, the CO and O reacts at the moment of their encounter in the same site. The cristalline structure of the surface suffers a phase transition that governs the dynamics of the problem, turning from a cubic 2-D lattice, when occupied by CO to an hexagonal one after desorption.

In this work we consider the simplest situation of only one *adsorbate*, with a lateral attractive interaction whose concentration is described by a scalar field, that is coupled to the phase transition process occuring on the surface. We model in a phenomenological way the processes associated with this scalar field that corresponds to:

- adsorption,
- desorption, including a local bounding associated to the lateral interaction,
- diffusion,
- a flux induced by the lateral interaction,
- reaction (modeled as a simple annihilation process).

Together with these aspects, we must also consider those related with the phase transition on the surface. This phenomenon, that must be dynamically coupled to the scalar field, is described using a Ginzburg-Landau functional for an order parameter associated to the phase on the surface. This coupled system resembles an activator-inhibitor one, but have additional characteristics associated to the flux induced by the lateral interaction.

We have stablished the phenomenological constraints that allows the existence of "bubbles" with a high density of the adsorbate, inmersed in an extended low density region. These conjetures have been tested, solving numerically the coupled set of equations for the density and the order parameter. The adopted numerical scheme was based in a path integral procedure that allows to transform the original set of partial differential equations into a set of selfconsistent integral equations. The same procedure was exploited to analyze the propagation of fronts and test the analytical results obtained via a singular perturbation approach.

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