Modeling of oscillatory behavior in heterogeneous catalysis: CO oxidation reaction

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The study of catalytic oxidation processes on Pt surfaces is of considerable interest since the apparently simple kinetics of this reaction can give rise to different types of behavior. Experiments have demonstrated the existence of a variety of non-linear phenonena such as nucleation induced front propagation, spiral wave dynamics, faceting structures and kinetic oscillations.

In this work we investigate some aspects of kinetic oscillations observed in the catalytic oxidation of CO on a Pt(110) surface at low pressures. For a kinetic model based on a Langmuir-Hinshelwood mechanism we have established that, at intermediate pressures, the system exhibits the first-order phase transition from a reactive state with medium O coverage to an inactive state, where the surface is predominantly covered by CO. This is the bistability phenomenon.

From the analysis of stability we have found few types of stationary points of the model which present different stability regimes, namely the stable and the unstable oscillatory ones. Oscillatory regime arises due to the interplay between bistability and adsorbate-induced surface reconstruction 1×2.