Catalytic CO oxidation reaction: lattice models and kinetic description

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The study of heterogeneous catalytic reactions have developed into a very active field of research in recent years. From the physical point of view, the kinetics of these reactions are of interest due to their richness and complexity related to such factors as surface heterogeneity, adsorbate-adsorbate lateral interactions, spontaneous and adsorbate-induced surface restructuring, and manifested in such phenomena as chemical waves, kinetic oscillations, and chaos.

Among the most studied reactions is the catalytic oxidation of carbon monoxide on platinum surfaces. Generally, catalytic CO oxidation reaction has been proven to proceed on Pt via a Langmuir-Hinshelwood mechanism in which both reactants are initially adsorbed on the surface. The goal of this work is to study catalytic CO oxidation on a Pt surface in the framework of a kinetic and a lattice-gas reaction models. On the basis of kinetic model we have found the stationary points of the system and analyzed them by their eigenvalues to reveal their stability. As it was found, at intermediate pressures the system exhibits two stable steady states, namely, a state of low reactivity with a predominantly CO covered surface, and a state of high reactivity with a largely oxygen-covered surface. The condition of the existence of the bistable region is analytically found and the bifurcation diagram is constructed. The effect of inactive impurities on the kinetics of catalytic reaction is studied. To give a more precise definition for model parameters, the ground-state phase diagrams of corresponding lattice models are investigated at temperature $T = 0$ by incorporating the nearest-neighbour interactions on a catalyst surface. The conditions of existence of nonuniform phases dependent on the interaction parameters are established and main types of ground-state phase diagrams are obtained.