Nonequilibrium Monte Carlo simulations applied to the ZGB model with CO desorption: A new look on its phase diagram

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In 1986, Ziff, Gullari, and Barshad proposed a model which simulates the oxidation of the carbon monoxide (CO) on a catalytic surface. In this model, which is now known as the Ziff-Gullari-Barshad (ZGB) model, the sites of a square lattice can be occupied by CO molecules, by oxygen (O) atoms, or be vacant (V). This model possesses only one control parameter, the CO adsorption rate $y$, and exhibits three distinct states and two irreversible phase transitions: one continuous and another discontinuous. The continuous transition occurs between the state where the lattice is completely filled with O atoms and the active phase where there is consistent production of carbon dioxide ($CO_2$). On the other hand, the discontinuous transition occurs between the active phase and the phase where all sites are occupied by (CO) molecules. Several modified versions of the model have been proposed in order to obtain more realistic systems of actual catalytic processes, for instance, by including CO desorption, diffusion, impurities, attractive and repulsive interactions between the adsorbed molecules, surfaces of different geometries, and with hard oxygen boundary conditions. In this work, we study the behavior of the phase transitions of the Ziff-Gullari-Barshad (ZGB) model when the CO molecules are adsorbed on the catalytic surface with a rate $y$ and desorbed from the surface with a rate $k$. We employ large-scale out-of-equilibrium Monte Carlo simulations, along with a technique known as coefficient of determination, to obtain a clue of the points $(y_c, k_c)$ where the first- and second-order phase transitions of the model take place when $y$ and $k$ vary. The simulations take into account the whole spectrum of $y$ and $k$: $(0 \leq y \leq 1$ and $0 \leq k \leq 1)$ with precision $\Delta y = \Delta k = 0.001$. Our results are compared with estimates found in literature.