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Monte Carlo study of surface reactions: I. Dimer–monomer irreversible reaction on partially deactivated surface

Badanie reakcji powierzchniowych metodą Monte Carlo:
I. Nieodwracalna reakcja dimer–monomer
na częściowo deaktywowanej powierzchni

1. INTRODUCTION

Surface catalyzed reactions occurring in open systems exhibit various kinetic (or nonequilibrium) phase transitions[1–4]. In general such processes are very complex and strongly affected by adsorption, desorption, diffusion and reaction rates[4–8]. One of the most intensively studied systems is the lattice model for the carbon monoxide oxidation on a single-crystal catalyst surface[4,8–15]. Experimental studies[16–18] have demonstrated that the carbon monoxide oxidation is a Langmuir–Hinshelwood process, and its basic steps are: i) adsorption of CO molecule on a single vacant site, ii) dissociative adsorption of O_2 molecule on a pair of adjacent empty sites, and iii) reaction between CO and O followed by desorption of the CO_2 molecule. Since the binding energy for CO is lower than the binding energy of oxygen atoms[19,20], the former undergoes surface diffusion during the process, while oxygen atoms are considerably less mobile.

From the numerous mean-field[5,9,13,14,21] and Monte Carlo[4,8,22–25] studies it follows that this system exhibits two kinetic phase transitions as the impingement rates of the reactants change. The model introduced by Ziff et al.[4] assumes

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the infinite reaction rate and no diffusion of the reactants. These authors have performed extensive Monte Carlo simulation for the impingement rate of CO molecules p_{CO} between 0 and 1 (the corresponding impingement rate for O_2 molecules is equal to $p_{O_2} = 1 - p_{CO}$. At low p_{CO} the poisoning of the surface by oxygen atoms occurs. As the probability of CO adsorption increases, however, the continuous transition between this O – poisoned and the reactive states occurs at p_{CO}^1 equal to 0.389. The reaction window spans the region of p_{CO} between p_{CO}^1 and $p_{CO}^2 = 0.525$. At p_{CO} equal to p_{CO}^2 the second, first-order transition occurs and for higher values of p_{CO} the CO-poisoned state appears. The locations of these phase transitions change when the diffusion of reactants is allowed[8,14,26], when the reaction rates are finite[8] as well as when the desorption of reactants can take place[4,21].

Another interesting problem is the influence of the catalyst surface nonuniformity on the reactions and the kinetic phase transitions. The presence of surface defects on the properties of reacting systems has been previously considered by many authors[27–30]. In particular, Monte Carlo simulations performed on percolating clusters and Sierpinsky carpet[29,30,31], both with the fractal dimension $D_F = 1.89$ have shown that the monomer–dimer reaction system exhibits two second-order (continuous) transitions, instead of one first-order and one second--order transition found for the two-dimensional systems (with $D_F = 2$). Effects of surface deactivation on the catalytic reactions have also been studied for the oxidation of methanol to CO on sulfur containing Fe(100)[32–34] and Ni(100) [35] surfaces. It has been shown that as the surface coverage of sulfur increases the production of CO considerably decreases and another reaction, leading to the formation of formaldehyde, takes precedence.

In this paper we consider a simple monomer–dimer reaction and discuss the effects of the reaction rate magnitude on the locations of the kinetic phase transitions and the changes in the mechanism of these transitions when the surface contains randomly distributed nonactive impurities.

2. THE MODEL AND MONTE CARLO METHOD

We consider a simple square lattice of the size $L \times L$ and assume that each lattice site is accessible for adsorbing molecules. The adsorbing mixture consists of two types of molecules A_2 (O_2) and B (CO). In general, we assume that only a certain fraction γ_a of the total number of sites (L^2) is active. These active sites

are assumed to be distributed randomly over the lattice. The particles B arrive at the surface with the probability p_B and the particles A_2 with the probability $p_{A_2} = 1 - p_B$. Adsorption of B occurs whenever the particle meets an empty site, while adsorption of A_2 requires a pair of adjacent empty sites. The state of the adsorbed B molecules is not affected by the type of adsorption site (active – marked by S^*, and nonactive – marked by S). On the other hand, the state of the adsorbed A_2 molecule depends on the type of sites. If both adsorbing sites are nonactive the A_2 molecule does not dissociate. When at least one of the adsorbing sites is active, however, the adsorption of A_2 is accompanied by dissociation. Only these atoms A which are adsorbed on active sites are able to react with B particles and form the product AB (CO_2) which immediately desorbs from the surface leaving two empty sites. The reaction rate is assumed to be finite and equal to k. Particles B, are assumed to be able to diffuse over the surface at the jump rate Γ_B independently of the lattice site type. Also the molecules A_2 and the atoms A adsorbed on nonactive sites can travel over the surface at the jump rates equal to Γ_{A_2} and Γ_A, respectively. The atoms A adsorbed on active sites (marked by A_a^*) remain localized, however. Whenever the diffusing adsorbed molecule A_2 meets an active site it dissociates into two A atoms.

Thus, the adsorption processes can be represented as

$$B^g + S \longrightarrow B^a \tag{1}$$

$$A_2^g + 2S \longrightarrow B_2^a \tag{2}$$

when both sites are nonactive,

$$A_2^g + 2S^* \longrightarrow 2A^{a*} \tag{3}$$

when both adsorbing sites are active (A^{a*} denotes adsorbed activated A atoms) and

$$A_2^g + S + S^* \longrightarrow A^a + A^{a*} \tag{4}$$

when only one of the adsorbing sites is active. The dissociative diffusion of A_2 molecules can be represented as

$$A_2^a + S^* \longrightarrow A^a + A^{a*} + S \tag{5}$$

Finally, the reaction occurs according to the equation

$$A^{a*} + B^a \longrightarrow AB^g + S^* + S(S^*) \tag{6}$$

and the product immediately leaves the surface.

To study the behavior of such systems we have used the Monte Carlo method. The applied algorithm is quite similar to that used previously by Sholl and Skodje[8]. Thus, we assume that a single Monte Carlo attempt can be adsorption of either A_2 or B particle (with the probabilities given by p_{A_2} and $p_B = 1 - p_{A_2}$, respectively, diffusion of B, diffusion of nondissocited A_2 molecule or A atom adsorbed on nonactive sites, or the reaction between A and B, accompanied by the desorption of the resulting AB molecule. Thus, a single Monte Carlo step defines a time unit as equal to

$$t_0 = 1 + \Gamma_B + \Gamma_{A_2} + \Gamma_A + 2k \tag{7}$$

Monte Carlo attempts. Calculations have been carried out for lattices of the size $L = 120$ and for γ_a ranging between 0.025 and 1. The number of Monte Carlo steps used in this study varied considerably with the parameters describing the process. In general, B poisoning occurs much more rapidly than the processes occurring in the reaction window and A poisoning[4]. In the case of reactive states the simulation required up to 10^5 moves before the steady state was reached. Then, another 10^4 Monte Carlo steps has been performed to calculate averages. In all cases, several independent runs have been performed and the final results have been obtained by averaging over these runs. In the case of partially nonactive surfaces, the surface configuration of active sites has been generated separately in each run. Standard periodic boundary conditions have been applied in both directions.

3. THE EFFECT OF REACTION RATE ON THE PHASE DIAGRAM

Here we consider the effect of the changes in the reaction rate on the location of both kinetic phase transitions in the case of completely active surface ($\gamma_a = 1$). Although the problems of difussion and reaction rates have been al-

ready considered in the literature[4–8,26,36–40], we have decided to include a brief discussion for completeness. The performed calculations have also served as a check for the correctness of our simulation algorithm and code.

In the systems with fully active surface, all the adsorbed A_2 molecules dissociate and are completely localized, while the molecules B are assumed to travel over the surface with the jump rate $\Gamma_B = 1$. Fig. 1 shows the changes in the reaction window, i.e., the locations of the kinetic phase transitions ($p^1_{A_2}$ and $p^2_{A_2}$, versus the reaction rate k. The result for $k = \infty$ has been taken from Ref. (4) and corresponds to the situation in which both reactants are fully localized.

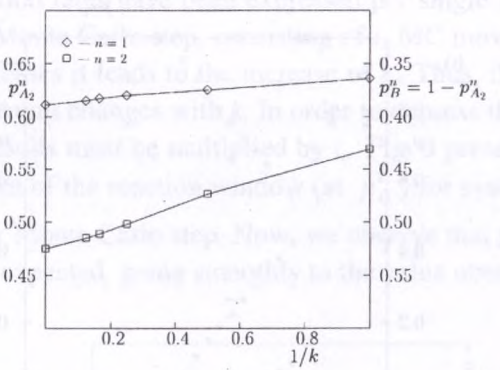

Fig. 1. Dependence of the kinetic phase transition points on the reciprocal reaction rate ($1/k$) for the systems with $\Gamma_B = 1$. Only the results for $k = \infty$ correspond to $\Gamma_B = 0$ and have been taken from Ref. (4)

Zależność między punktami kinetycznej przemiany fazowej i odwrotnością stałej szybkości reakcji ($1/k$) w przypadku układów z $\Gamma_B = 1$. Jedynie wyniki otrzymane dla $k = \infty$ odpowiadają $\Gamma_B = 0$ i zostały zaczerpnięte z pracy (4)

We observe that as the reaction rate becomes smaller the reaction window becomes narrower, mostly due to rather large change in the location of the first order kinetic phase transition $p^2_{A_2}$. The continuous transition separating reactive and B-poisoned states is only very slightly affected by the reaction rate. Also, the diffusion of reactants has a small influence on the reaction window when the reaction rate is high. On the other hand, for small reaction rates the increase in the jump rate of the reacting particles is expected to be more important[8,14].

In Fig. 2 we present the examples of phase diagrams for the systems characterized by $k = 1$, 2 and 4, and the jump rate for the component B equal to $\Gamma_B = 1$. Our results for $k = 1$ are the same as reported earlier by Sholl and

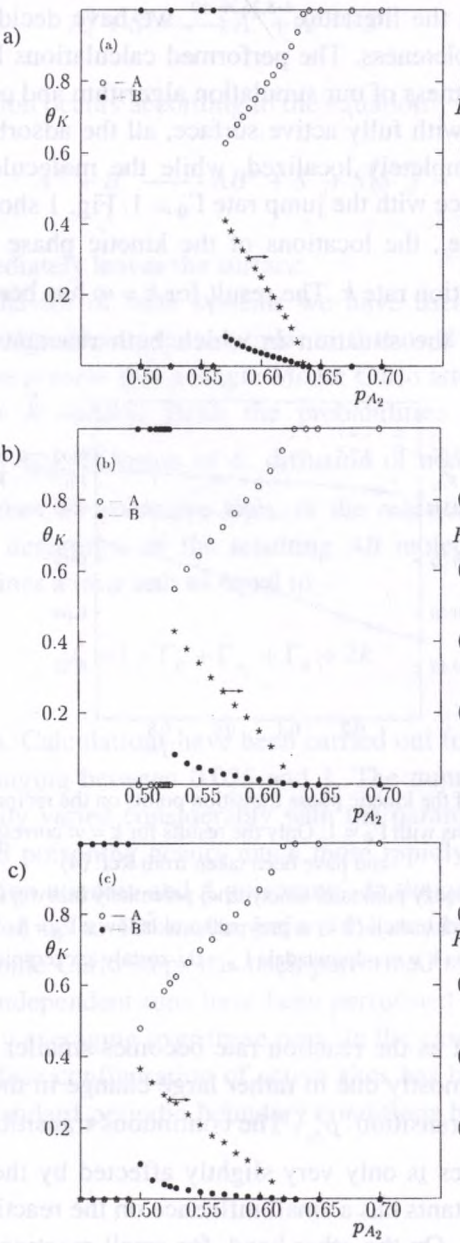

Fig. 2. Phase diagrams for the systems with $k = 1$ (part (a)), $k = 2$ (part (b)) and $k = 4$ (part (c)), obtained for the model with $\Gamma_B = 1$

Diagramy fazowe odpowiadające układom z $k = 1$ (część a), $k = 2$ (część b) oraz $k = 4$ (część c) odpowiadające modelowi z $\Gamma_B = 1$

Skodje[8]. In particular, we have found that the kinetic data in the region of *B*-poisoning transition approximately obey the scaling relations

$$\theta_B(t) = F\left[(p_{A_2}^{s1} - p_{A_2})t\right] \tag{8}$$

$$\theta_A(t) = F\left[(p_{A_2}^{s1} - p_{A_2})t\right] \tag{9}$$

where $p_{A_2}^{s1}$ represents the location of the spinodal point.

The results for the production rate, presented in Fig. 2, require some comments. The production rates have been expressed per single Monte Carlo move and not per single Monte Carlo step, consisting of t_o MC moves. As the reaction rate constant k increases it leads to the increase of t_o. Thus, the number of reaction events per time unit changes with k. In order to express the production rates per MC step, the results must be multiplied by t_o. Fig. 3 presents the production rates just at the onset of the reaction window (at $p_{A_2}^2$) for systems with different k and expressed per Monte Carlo step. Now, we observe that the production rate increases with k as expected, going smoothly to the value obtained for $k = \infty$.

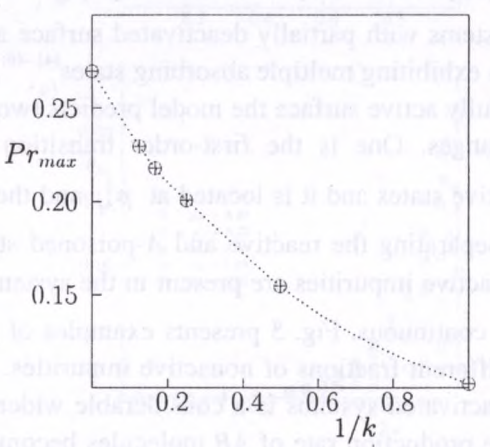

Fig. 3. The maximum production rate at the onset of the reaction window at $p_{A_2}^2$ as a function of the reciprocal reaction rate, for the systems with $\Gamma_B = 1$. Results for $k = \infty$ have been taken from Ref. (4)

Maksima szybkości produkcji w punktach początkowych okna reakcji $p_{A_2}^2$ jako funkcja odwrotności stałej szybkości reakcji w przypadku układów z $\Gamma_B = 1$. Wyniki odpowiadające $k = \infty$ zaczerpnięto z pracy (4)

4. REACTION ON PARTIALLY DEACTIVATED SURFACE

For small values of p_{A_2} (lower than $p^1_{A_2}$) and when all sites are active the surface becomes *B*-poisoned, i.e., entirely covered by the adsorbed *B* particles. When the fraction of active sites becomes lower than unity, we also observe poisoning, but with nonzero concentrations of *B* and both A_2 and *A* particles. This is illustrated in Fig. 4, which presents the surface coverages of *A*, A_2 and *B* particles in the steady state for surfaces characterized by different fraction of nonactive impurity sites ($\gamma_{na} = 1 - \gamma_{na}$). The total surface coverage is very close to unity in all cases, however. Note that the surface coverage of nondissociated A_2 molecules is given by the ratio $\theta_{A_2} = N_{A_2}/L^2$, where N_{A_2} is the number of A_2 molecules in the system. Thus, the number of sites occupied by A_2 molecules is equal to $2N_{A_2}$. The presence of *A* atoms results from the fact that some of them are trapped on nonactive sites and surrounded by either nondissociated A_2 or *B* molecules. According to the assumed model, the atoms *A* adsorbed on nonactive sites do not react with *B* molecules. As the fraction of nonactive sites goes to unity, the reaction ceases completely and the surface becomes covered by A_2 and *B* particles in the proportions fully determined by p_{A_2}. It is obvious that the considered here systems with partially deactivated surface are examples of the well-known models exhibiting multiple absorbing states[41–48].

In the case of fully active surface the model predicts two kinetic phase transitions as p_{A_2} changes. One is the first-order transition separating the *B*-poisoned and reactive states and it is located at $p^2_{A_2}$ and the second is the continuous transition separating the reactive and *A*-poisoned states and located at $p^1_{A_1}$. When the nonactive impurities are present in the system, we find that both transitions become continuous. Fig. 5 presents examples of phase diagrams for the systems with different fractions of nonactive impurities. An interesting feature of partially deactivated systems is a considerable widening of the reaction window, though the production rate of *AB* molecules becomes lower and lower as the fraction of nonactive sites increases. When the production rate is related to the number of active sites only and not to the total number of sites, we find that the maxima of the production rate for partially deactivated surfaces appear at different values of p_{A_2} for a given fraction of active sites γ_a.

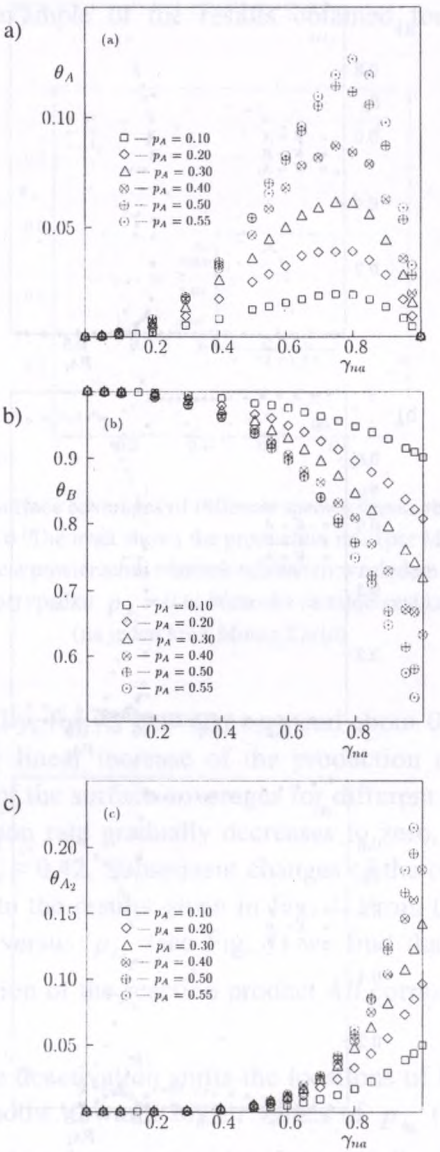

Fig. 4. Surface coverages of species A (part (a)), B (part (b)) and A_2 (part (c)) for partially deactivated surfaces and different values of p_{A_2} below the first-order kinetic phase transition, for the systems with $k = 1$, $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$

Stopnie pokrycia powierzchni substancji A (część a), B (część b) oraz A_2 (część c) odpowiadające częściowo deaktywowanym powierzchniom i różnym wartościom p_{A_2} poniżej punktu kinetycznej przemiany fazowej pierwszego rzędu w przypadku układów z $k = 1$, $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$

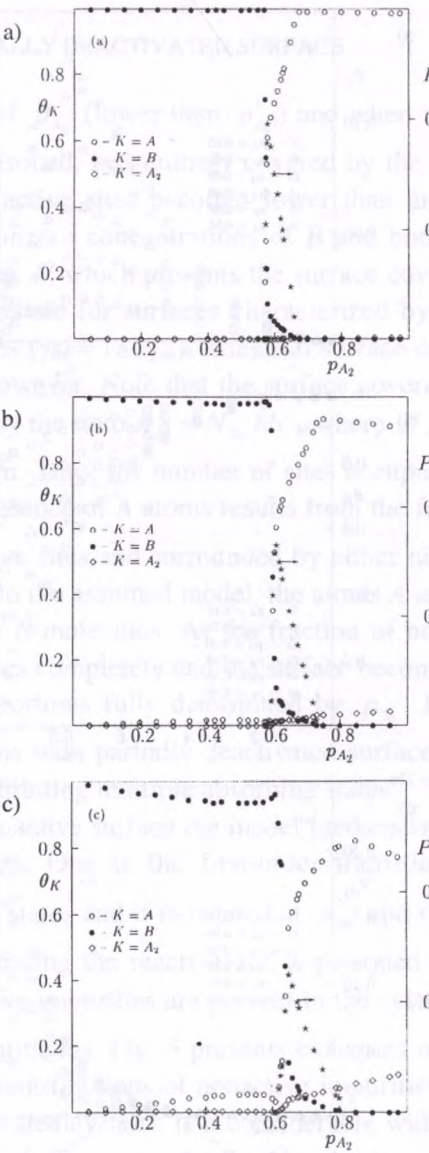

Fig. 5. Examples of phase diagrams for systems with partially deactivated surface with $\gamma_a = 0.9$ (a), 0.7 (b) and 0.5 (c). All results have been obtained for $k = 1$ and $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$

Przykłady diagramów fazowych odpowiadających układom z częściowo deaktywowaną powierzchnią z $\gamma_a = 0{,}9$ (a), 0,7 (b) i 0,5 (c). Wszystkie wyniki uzyskano w przypadku $k = 1$ i $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$

Fig. 6 presents the example of the results obtained for p_{A_2} equal to 0.6.

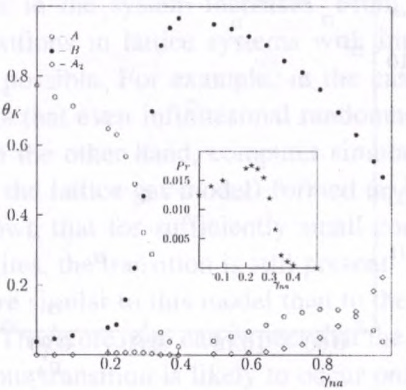

Fig. 6. The changes in the surface coverages of different species versus the degree of surface deactivation for $p_{A_2} = 0.6$. The inset shows the production rate (per Monte Carlo move)

Zmiany stopnia pokrycia powierzchni różnych substancji względem stopnia deaktywacji powierzchni w przypadku $p_{A_2} = 0.6$. Wstawka ukazuje szybkości produkcji (na jeden krok Monte Carlo)

We observe that initially, for γ_{na} between zero and about 0.225, surface deactivation leads to nearly linear increase of the production rate and also causes nearly linear changes of the surface coverages for different species. Then, as γ_{na} increases, the production rate gradually decreases to zero, and the surface becomes poisoned for $\gamma_{na} \approx 0.42$. Subsequent changes of the coverages for all species are quite similar to the results given in Fig. 4. From the plot of the maximum production rate versus p_{A_2} (see Fig. 7) we find that the most optimum regime for the production of the reaction product *AB* corresponds to $p_{A_2} \approx 0.65$ and $\gamma_a \approx 0.8$.

In general, surface deactivation shifts the locations of both transitions, and hence the reaction window, towards higher values of p_{A_2} (see Fig. 8). We find that the reaction window becomes wider for partially deactivated surface, though the *AB* production rate rapidly decreases when the degree of surface deactivation increases.

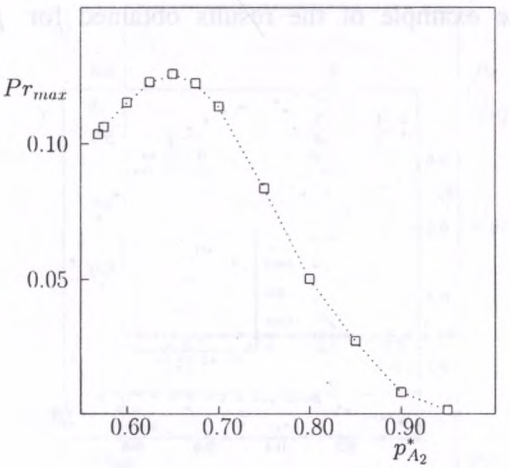

Fig. 7. The maximum production rate for partially deactivated systems as a function of p_{A_2} ($k = 1, \Gamma_A = \Gamma_B = 1, \Gamma_{A_2} = 1$)

Maksima szybkości produkcji w przypadku częściowo deaktywowanych powierzchni jako funkcja p_{A_2} ($k = 1, \Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$)

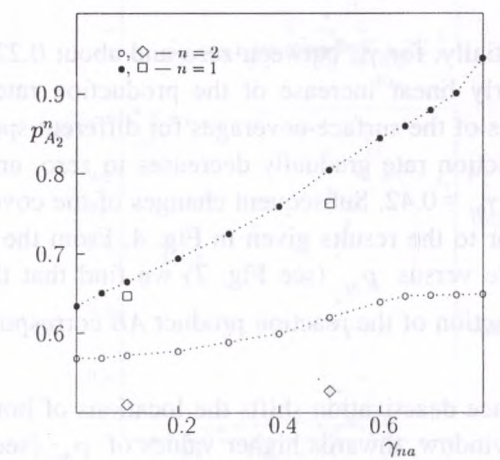

Fig. 8. Locations of the transition points in partially deactivated systems with $k = 1$ and $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$.

◊ and □ represent the results obtained for $k = 4$ and $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$

Położenie punktów przemiany fazowej w przypadku układów z częściowo deaktywowaną powierzchnią przy $k = 1$ i $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$.

◊ i □ odpowiadają wynikom uzyskanym w przypadku $k = 4$ i $\Gamma_A = \Gamma_B = \Gamma_{A_2} = 1$

An interesting problem that has not been considered here in detail, is the crossover between the first-order and continuous transition as the concentration of nonactive impurities in the system increases. From theoretical studies of equilibrium phase transitions in lattice systems with impurities[49–51] it follows that two scenarios are possible. For example, in the case of the random field Ising model one expects that even infinitesimal randomness destroys any sharp phase transition[49,50]. On the other hand, computer simulations for the adsorbed films (also modeled by the lattice gas model) formed on lattices containing two types of sites have shown that for sufficiently small concentration of less (or more) active impurity sites, the transition is still present[51]. The situation considered in this work is more similar to this model than to the above mentioned random field Ising model. Therefore, one can expect that the crossover between the first-order and continuous transition is likely to occur only for sufficiently high concentration of nonactive sites. Our results obtained for $\gamma_{na} = 0.05$ do not show any rounding of the first-order kinetic transition, while for $\gamma_{na} = 0.1$ the transition appears to be continuous.

Another emerging question is the effect of impurities on the critical behavior of the continuous kinetic phase transition occurring at $p^1_{A_2}$. In the case of fully active surface and infinite reaction rate, the critical properties of the considered model are well known[25,26]. It has been found that this transition belongs to the universality class of the directed percolation model[52]. The order parameter for this transition, θ_B, is expected to behave as

$$\theta_B(p_A) = \propto \left| p_A - p^1_A \right|^{\beta} \tag{10}$$

with the exponent β equal to 0.58. One can expect that surface deactivation should considerably affect this transition, or destroy it completely. Our results suggest that for sufficiently highly deactivated surface this transition becomes gradual, i.e., it is not any true phase transition any more (cf Fig. 5). In particular, it seems that the power-law given by eqn. (10) is not obeyed. In order to address this problem, and obtain more reliable results, the simulations for much larger systems are needed, however. In particular, the method developed to study damage spreading at equilibrium phase transitions[53], seems quite well suited for such problems[25] and will be considered in our future work, where we shall also present the solutions of the mean field equations for the model considered here.

Although, the considered model is extremely simple and the presented results have been obtained for rather small systems, but we believe that it is a

good starting point for investigation of more complex systems. In particular, it is possible to consider the situations in which there are several possible reactions occurring at the surface which compete one with another depending on the state of adsorbed species. Our preliminary results demonstrate that the production rate strongly depends on the surface activity and that surface deactivation may lead to an increase in the reaction yield (per one active site) in some cases. It is probably due to the assumed mobility of dimer molecules adsorbed on nonactive sites. The considered situation is somewhat similar to the model allowing diffusion of the dissociated A_2 particles over the surface. We shall return to this problem in our future work.

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STRESZCZENIE

Przedstawiono wyniki symulacji Monte Carlo dla modelowej, katalizowanej powierzchniowo reakcji $A_2 + 2B \rightarrow 2AB$. Rozważono wpływ zmian szykości reakcji oraz deaktywacji powierzchni na kinetyczne przemiany fazowe. Pokazano, że deaktywacja powierzchni katalizatora w istotny sposób wpływa na położenie okna reakcji oraz na mechanizm obserwowanych przemian fazowych. W szczególności, pokazano, że deaktywacja powierzchni zmienia rząd kinetycznej przemiany fazowej w kierunku przemiany ciagłej.