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Critical behaviour of continuous phase transitions with infinitely many absorbing states

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Abstract

A lattice gas model is proposed for the $A_2 + 2B_2 \rightarrow 2B_2A$ reaction system with particle diffusion. In the model, A_2 dissociates in the random dimer-filling mechanism and B_2 dissociation is in the end-on dimer-filling mechanism. A reactive window appears and the system exhibits a continuous phase transition from a reactive state to a covered state with infinitely many absorbing states. When the diffusion of particle A and AB is included, there are still infinitely many absorbing states for the continuous phase transition, but it is found that the critical behaviour changes from the directed percolation (DP) class to the pair contact process with diffusion (PCPD) class.

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1. Introduction

Recently, a study on the pair contact process with diffusion (PCPD) or annihilation fission process (AF) $2A \rightarrow \emptyset$, $2A \rightarrow 3A$ suggested that the diffusion of the particles should introduce a new kind of critical behaviour which is different from the well known universality classes [1–7]. Although the model has attracted much attention in the past few years, it is not yet clear whether its critical behaviour presents an independent universality class [8]. This model without the diffusion was first investigated by Jensen and the critical behaviour of the continuous phase transition with infinitely many absorbing states belongs to the directed percolation (DP) class [9]. When the particle diffusion is introduced, there are only two absorbing states: one is a vacuum state and another is that there is only one particle which can diffuse in the whole system.

In the present paper, we investigate a lattice gas model for the $A_2 + 2B_2 \rightarrow 2B_2A$ reaction system with particle diffusion on a heterogeneous catalytic surface. The dimer–dimer surface reaction system has been investigated on the basis of the well-known Langmuir–Hinshelwood mechanism [10, 11], no reactive window has been found if the desorption of the adsorbed B

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atom is ignored. In the previous lattice models, the dimer adsorbing trial is in the random dimer filling mechanism, in which a pair of nearest-neighbour (NN) sites is selected randomly for the dimer adsorption [12–16]. Therefore, the configuration of the adsorbate on surface does not affect the selection of a pair. However, for an actual reaction on surface, an adsorption process of a dimer involves in a very complicated dissociation on surface, and its dissociation depends on the surrounding chemical environment. Some authors have studied another dissociation mechanism of a dimer [16–20], which is called ‘end-on dimer filling’ mechanism where one end of the dimer adsorbs on a vacant site firstly and then the dimer can occupy another vacant site and dissociate into two atoms if there is one vacant NN site for the first site. Therefore, the selection of a pair for the dimer adsorbing trial is no longer purely random because the configuration of the adsorbate on the catalytic surface significantly affects the selection [20]. It is obvious that the adsorption probability for a dimer increases in the end-on mechanism and then it can take an important influence on the dynamical behaviour of the surface reaction system.

In our model, A_2 dissociates in the random dimer filling mechanism but B_2 dissociation is in the end-on dimer filling mechanism. A reactive window appears and the system exhibits a continuous phase transition with infinitely many absorbing states from a reactive state to an ‘A + AB + vacancy’ covered state. When the particle diffusion is included, there are still infinitely many absorbing states for the continuous phase transition, but the critical behaviour changes from the DP class into the PCPD class.

2. Model and simulation algorithm

We model the catalytic surface by a square lattice, which is in contact with an infinite reservoir of the two types of dimer, labelled here by A_2 and B_2 . These dimers can be adsorbed onto the lattice and dissociate into two atoms, which occupy two NN sites of the lattice, and they can react according to the following steps:

- (1) $A_{2(g)} + 2v \rightarrow 2A_{(ads)}$
- (2) $B_{2(g)} + 2v \rightarrow 2B_{(ads)}$
- (3) $A_{(ads)} + B_{(ads)} \rightarrow AB_{(ads)} + v$
- (4) $AB_{(ads)} + B_{(ads)} \rightarrow B_2A(g) + 2v$

in which the subscript ‘(g)’ denotes a species in gas phase and ‘(ads)’ indicates the adsorption state of a species on the lattice surface. Here ‘v’ indicates a vacant site on the lattice surface.

In our system, the dimer dissociation can follow one of the two mechanisms, which are random and end-on dimer filling mechanism. For the random dimer filling mechanism, first randomly pick one site, (if empty) then randomly select a NN site from the four NN sites, the dimer fills only if both sites are empty. As a result, a pair of two NN sites is selected randomly for the dimer adsorption.

The end-on dimer filling mechanism: first randomly pick one site, ‘i’, and if ‘i’ and at least one of the four NN sites are empty, choose another site randomly only from the empty NN sites. The dimer occupies the pair of two empty sites. Therefore, the selection of a pair for the dimer adsorbing trial is no longer purely random.

The adsorption–reaction process begins with a random collision of a gas molecule on an $L \times L$ square lattice. The colliding molecule is chosen to be a dimer B_2 with a given probability y_B which is the fraction of B_2 in gas phase and a dimer A_2 with a probability $1 - y_B$. If a dimer A_2 is adsorbed successfully, then check the six NN sites, the adsorbed A atom reacts with a B atom on a NN site to form AB on the site occupied by A, AB also can immediately react with a B atom on its NN sites to form a B_2A molecule which desorbs at

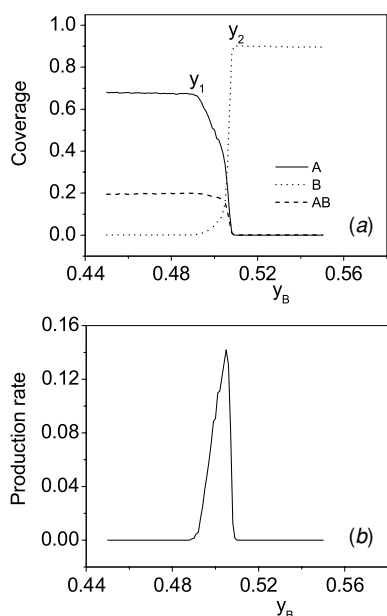


Figure 1. (a) The Monte Carlo simulation result of the coverage of A, B and AB against the fraction y_B ; (b) production rate of B_2A against y_B , $d = 0.0$.

once and leaves two vacant sites. If a dimer B_2 is adsorbed successfully, B atom can react with A or AB to form AB or B_2A , then there are three possibilities (a) formation of B_2A is prior to the formation of AB, (b) formation of AB is prior to the formation of B_2A and (c) both formations have an equal probability. In present work, we have taken the first case. In reality, from our simulation results and previous works [10, 11], the difference of the three reaction paths has little influence on the kinetic behaviour.

For the particle diffusion process, a site is chosen randomly; if it is occupied by a particle, then a NN site is selected randomly; if this NN site is vacant, then the particle jumps to this site and the corresponding reaction step of the particle can occur at once as described above.

In our simulation, A_2 dissociates in the random dimer filling mechanism but B_2 dissociation is in the end-on dimer filling mechanism and the diffusion of particle A and AB is included.

At the beginning of a simulation step, a random number ρ_0 between 0.0 and 1.0 is generated. A diffusion attempt ($\rho_0 < d$) or an adsorption–reaction process ($\rho_0 > d$) is performed, respectively, where d indicates the particle diffusion probability. We take our simulation on a lattice 128×128 with a periodic boundary condition and an initial empty surface.

3. Simulation results and discussion

When the particle diffusion is ignored, the simulation result is shown in figure 1. For a y_B value, the simulation results are averaged over 400 independent samples and a sample runs 5000 Monte Carlo steps (MCS) (a MCS means a Monte Carlo attempt for every lattice site). From figure 1, it is found that there are two phase transitions at y_1 and y_2 . When $y_B < y_1$, the surface is covered by A, AB and isolated vacancies eventually and the reaction ends. When $y_B > y_2$, the surface eventually is covered by B and isolated vacancies and the reaction ends also. Between y_1 and y_2 , there are A, AB, B and pair of vacant sites on the

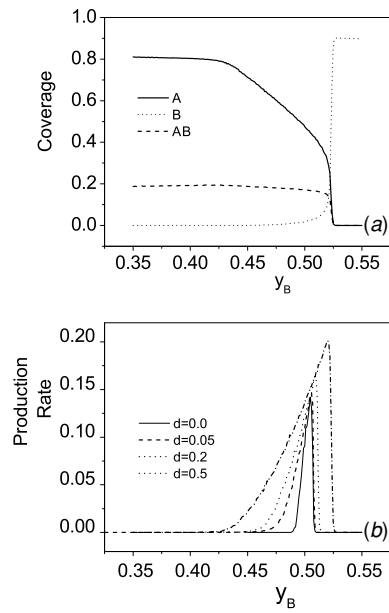


Figure 2. (a) The Monte Carlo simulation result of the coverage of A, B and AB against the fraction y_B ($d = 0.50$); (b) production rate of B_2A against y_B under different diffusion probability.

surface and then the reaction can continue. The system exhibits a continuous phase transition at y_1 from an active reaction state to an ‘A + AB + vacancy’ covered state and a discontinuous phase transition at y_2 to a ‘B + vacancy’ covered state.

It is obvious that there are infinitely many absorbing states for the continuous phase transition when the lattice size tends to infinity. We have investigated the critical behaviour by calculating the ratio of static critical exponents with Monte Carlo simulation¹ and the critical behaviour belongs to the DP universality class as we expected [17–20].

When the diffusion of the particle A and AB is considered, the simulation results are shown in figure 2. With the diffusion probability increasing, the continuous transition point decreases but the discontinuous transition point increases, then the width of the active reaction window increases. It is obvious that, for the continuous phase transition, there are still infinitely many absorbing states of A + AB. Due to the PCPD problem mentioned above, the influence of the particle diffusion on the critical behaviour of the continuous phase transition is very interesting.

As we know, the upper critical dimension for the PCPD model is two dimensions [8]. Therefore, we investigate the critical behaviour of the continuous phase transition with mean field theory including the particle A and AB diffusion process. According to the site approximation method [21], we ignore all spatial correlations and obtain the evolution equation as below:

$$\frac{dP_A}{dt} = 2y_A(1-d)P_V^2(1-P_B)^3 - 2y_B(1-d)P_V[1 - (1-P_V)^4][P_A(1-P_{AB})^2 + P_A^2(1-P_{AB}) + P_A^3] - dP_AP_V[1 - (1-P_B)^3] \quad (1)$$

¹ When the diffusion process is neglected, defining the order parameter ρ = per cent of pairs of vacant sites, we can estimate the transition point and the ratio of two static critical exponents by Monte Carlo simulation simply, $y_1 = 0.4938 \pm 0.0002$, $\beta/\nu_\perp = 0.81 \pm 0.01$, $\beta/\nu_\parallel = 0.45 \pm 0.01$.

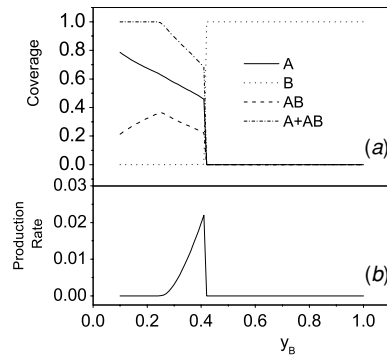


Figure 3. The numerical integration result from the mean field equations (1)–(3): (a) the coverage of A, B and AB against y_B ; (b) production rate of B_2A ($d = 0.8$).

$$\begin{aligned} \frac{dP_B}{dt} = & 2y_B(1-d)P_V[1-(1-P_V)^4](1-P_A-P_{AB})^3 \\ & - 2y_A(1-d)P_V^2[P_B(1-P_B)^2 + 2P_B^2] \\ & - dP_AP_V[P_B(1-P_B)^2 + 2P_B^2] - dP_{AB}P_V[1-(1-P_B)^3] \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{dP_{AB}}{dt} = & 2y_A(1-d)P_V^2(1-P_B)^2P_B + 2y_B(1-d)P_V[1-(1-P_V)^4][P_A(1-P_{AB})^2 \\ & + P_A^2(1-P_{AB}) + P_A^3] - 2y_B(1-d)P_V[1-(1-P_V)^4][1-(1-P_{AB})^3] \\ & + dP_AP_VP_B(1-P_B)^2 - dP_{AB}P_V[1-(1-P_B)^3] \end{aligned} \quad (3)$$

where $y_A + y_B = 1$, P_A , P_B , P_{AB} and P_V are the coverage of particle A, B, AB and vacant site on surface, respectively. $P_A + P_B + P_{AB} + P_V = 1$, d is the diffusion process probability. In equation (1), the first term describes the coverage increase of particle A because of A_2 adsorption, the second term describes the coverage decrease of particle A because of B_2 adsorption and third term means the coverage decrease of particle A due to A diffusion and reaction with particle B. We can obtain equations (2) and (3) in a similar way.

Although the mean field theory implies that a particle may meet all of the other particles with an equal probability which means a rapid particle diffusion, the evolution equation still includes the diffusion terms of particle A and AB because a reaction process may occur after the diffusion process of A and AB particle. In fact, the diffusion terms in the equations have no effect on the critical behaviour of the continuous phase transition except the production rate under the site approximation condition. The production rate is $2y_A(1-d)P_V^2P_B^2 + 2y_B(1-d)P_V[1-(1-P_V)^4][1-(1-P_{AB})^3] + dP_AP_VP_B^2 + dP_{AB}P_V[1-(1-P_B)^3]$, the beginning two terms describe the contribution of A_2 and B_2 adsorption processes to the reaction rate respectively, the last two terms denote the contribution of A and AB diffusion processes.

From equations (1)–(3), $P_V = 0$ is a poisoned steady state. Following a numerical integration of equations (1)–(3) with an empty initial condition under different y_B , we can obtain the transition behaviour with y_B varying. The calculation result is shown in figure 3. For every y_B value, the numerical integration continues until the system enters into a stationary state. We can see that the mean field theory predicts the continuous phase transition and the discontinuous phase transition very well which are in consistence with the Monte Carlo simulation results in figures 1 and 2, although the two critical points are not predicted accurately.

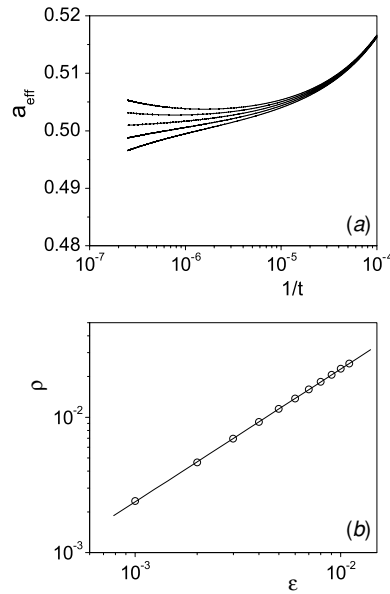


Figure 4. (a) Local slope of the order parameter $\rho(t)$ decay for $y_B = 0.25001, 0.250005, 0.250000, 0.249995, 0.249990$ (from bottom to top) from equations (1)–(3); (b) the double logarithmic plot for ρ versus ε ($\varepsilon = y_B - y_c$) ($d = 0.8$).

Considering the particle diffusion process, two isolated vacant sites can meet together to form a pair of vacancies and then the reaction can continue. From figure 3(a), we can define an appropriate order parameter $\rho = 1 - P_A - P_{AB}$. According to the local slopes of order parameter $\rho(t)$ to estimate the critical point, we define the decay exponent $\alpha_{\text{eff}}(t)$: $\alpha_{\text{eff}}(t) = \frac{-\ln[\rho(t)/\rho(t/m)]}{\ln(m)}$, where m is an integer number, in our calculation $m = 10$. We can calculate the decay critical exponent of the order parameter and the continuous transition point y_c following the numerical integration of equations (1)–(3). As shown in figure 4(a), we can obtain $\alpha_{\text{eff}} = 0.5 \pm 0.005$ and $y_c = 0.250000 \pm 0.000005$. Furthermore, we can define the order parameter exponent: $\rho \propto (y_B - y_c)^\beta$. Following the numerical integration of equations (1)–(3) in the adjacency of the transition point y_c , we measure the order parameter ρ from the stationary state, then we can estimate $\beta = 0.98 \pm 0.02$ from the results in figure 4(b). It is shown that the critical behaviour of the continuous phase transition belongs to the PCPD class when the particle diffusion is considered. On the other hand, we show a double-logarithmic plot of $\rho(t)t^{0.5}$ as a function of t in figure 5, the pronounced downward curvature of the data in the double-logarithmic plot discloses a strong long time logarithmic correction to scaling [3], but the numerical integration over 10^6 helps to estimate the critical point and the decay exponent accurately which are in consistency with the results in figure 4(a).

There are still infinitely many absorbing states for the continuous phase transition after the particle diffusion is introduced, but they can be divided into two subsets, one is that there is no vacant site on the surface and another is that there is only one vacant site. The structure of the infinitely many absorbing states is changed and the critical behaviour changes from the DP universality class to the PCPD class.

In conclusion, we investigate a lattice gas model for the $A_2 + 2B_2 \rightarrow 2B_2A$ reaction system in two dimensions. A_2 dissociates in the random dimer-filling mechanism but B_2

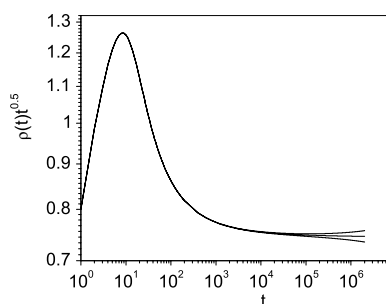


Figure 5. The double logarithmic plot $\rho(t)t^{0.50-t}$ for $y_B = 0.24999, 0.25000, 0.25001$ (from bottom to top) ($d = 0.8$).

dissociation is in the end-on dimer filling mechanism. A reactive window appears and the system exhibits a continuous phase transition with infinitely many absorbing states from a reactive state to an ‘A + AB + vacancy’ covered state and a discontinuous phase transition to a ‘B+vacancy’ covered state. When the diffusion of particle A and AB is included, there are still infinitely many absorbing states for the continuous phase transition, but they can be divided into two subsets. It is found that the critical behaviour changes into the PCPD class.

Acknowledgments

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