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Monte Carlo simulation of ramified aggregates on hetero-substrates*

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We have studied the aggregation of particles on a hetero-substrate consisting of two different substrates A and B with finite surface barriers $E_{\rm AB}$ and $E_{\rm BA}$ between the AB and BA boundaries, respectively. With the diffusion energy limited aggregation (DELA) model, we find that the number of clusters and the mean radius of gyration of the clusters are dependent on the surface barriers $E_{\rm AB}$ and $E_{\rm BA}$. For the case with a constant of $E_{\rm BA}$, a series of minima are summarized as $E_{\rm AB} = (E_0 - k_{\rm BA}E_{\rm BA})/k_{\rm AB}$ with $k_{\rm AB}$ and $k_{\rm BA}$ being two integers, for main minima ($k_{\rm BA} = k_{\rm AB} - 1$) and two local minima ($k_{\rm BA} = k_{\rm AB}$ and $k_{\rm BA} = k_{\rm AB} + 1$) between two neighbouring main minima.

Keywords: diffusion energy limited aggregation, hetero-substrate, Monte Carlo simulation, cluster
PACC: 6855, 0555, 6870

1. Introduction

The computer simulation of thin film growth has been an important issue in surface physics.[1−4] With computer simulations, one can set up a model system to check the correctness of thin film growth theories. A lot of computer simulation models such as the diffusion limited aggregation (DLA) model,[5] the cluster-cluster aggregation (CCA) model,[6,7] the deposition diffusion aggregation (DDA) model,[8] the deposition diffusion rotation aggregation (DDRA) model[9] etc., were established to explain different aggregation phenomena of atoms on substrates. Though they and their developments assumed an ideal surface in the models, many excellent results have been obtained.[10−16] However, impurities or defects always exist on the material surfaces in practical physical systems.[17,18] For some special situations, one needs to introduce impurity atoms or atomic clusters into clean substrates as a nucleus of aggregation.[19,20] Moreover, in many cases, the substrates are composed of different materials (the crystal surface with a quantum dot array, for instance). Therefore, the diffusion coefficient of the deposited atoms changes in the different substrate regions,[21] or the atoms need to overcome energy barriers when they diffuse across the boundaries.[22,23] It was found that, after gold atoms deposited on a molten glass substrate with impurities distributed randomly, they could only diffuse and aggregate outside of the impurity regions. Therefore, the final ramified aggregations may exhibit characteristic microstructures.[24,25]

In this work, we study the aggregation of particles (or atoms) on a hetero-substrate which is composed of two different substrates A and B. Particles not only consume energy $E_{\rm A}$ (or $E_{\rm B}$) when they move one lattice forwards on substrate A (or B), but also consume energy $E_{\rm AB}$ (or $E_{\rm BA}$) when they pass through the boundary from A to B (or from B to A). The growth of ramified aggregations on a hetero-substrate surface is simulated using the diffusion energy limited aggregation (DELA) model for a square lattice. The simulation results illustrate that the aggregation highly depends on the values $E_{\rm AB}$ and $E_{\rm BA}$. A law that governs the aggregation properties, such as the number of clusters and mean radius of gyration, is discovered.

2. The diffusion energy limited aggregation (DELA) model

Computer simulations are carried out on a square lattice with size $L \times L$. There are several small squares with size $L_{\rm B} \times L_{\rm B}$ periodically distributed on the square lattice. These small squares are named as substrate B to distinguish them from the left area named

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substrate A. Substrates A and B have different physical properties, therefore the system is called a hetero-substrate. The system is periodic in both x and y directions. All the deposited particles are identical and can only sit on lattice sites. The particle consumes energy $E_{\rm A}$ when it moves one lattice unit on the substrate A, and $E_{\rm B}$ on the substrate B. When it passes through the boundary of two substrates, it consumes energy $E_{\rm AB}$ moving over the boundary from A to B and $E_{\rm BA}$ from B to A. Figure 1 shows the system for simulations.

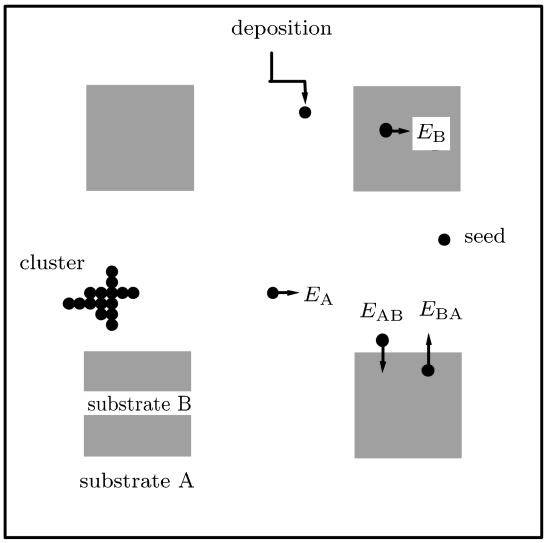


Fig.1. Schematic diagram of the hetero-substrate model on a square lattice. The parts of substrate B (grey squares) are arranged periodically on the square lattice, while substrate A (white) occupies the remainder of the space.

We adopt the DELA model, in which a total of n particles are deposited on vacant positions in sequence. That is, the next particle is deposited immediately after the previous one is stopped. Each particle has an initial kinetic energy E_0. In every simulation step the particle deposited moves one step, i.e., one lattice unit in one of the four possible directions ($\pm x$, $\pm y$) randomly. A particle stops if it uses up its initial kinetic energy E_0, or it reaches a site adjacent to other particles or clusters. For the former situation the stopped particle is then called the seed. In this paper, both seed and clusters are named as cluster for convenience. If two clusters touch each other, then they will irreversibly adhere to each other and a larger cluster is thus formed.

3. Result and discussion

Simulations are carried out on the square lattice with 400×400 lattice sites. We first examine the final morphologies for two limitations: (1) $E_{\rm AB} = E_0$, $E_{\rm BA} = 0$, and (2) $E_{\rm BA} = E_0$, $E_{\rm AB} = 0$. For the first case, the particle cannot walk through the boundary from A to B since $E_{\rm AB} = E_0$, while it can freely walk though the boundary in the opposite direction. For the second case, the particle cannot walk through the boundary from B to A for $E_{\rm BA} = E_0$. The initial kinetic energy is set to be $E_0 = 20000$ and the total particle number is $n = 20000$. For the first case ($E_{\rm AB} = E_0$), only a very small amount of particles is in the substrate B (Fig.2(a)). Here the size of square B is $L_{\rm B} = 20$, and the number of square B is $M = 25$. On the contrary, for the second case ($E_{\rm BA} = E_0$), a large amount of particles is on the substrate B. When the area of substrate B is larger than the number of particle B ($M = 100$ and $L_{\rm B} = 20$ used in Fig.2(b)), we find that most of particles are on the substrate B as shown in Fig.1(b). This may bring a new way to control the position of deposited particles.

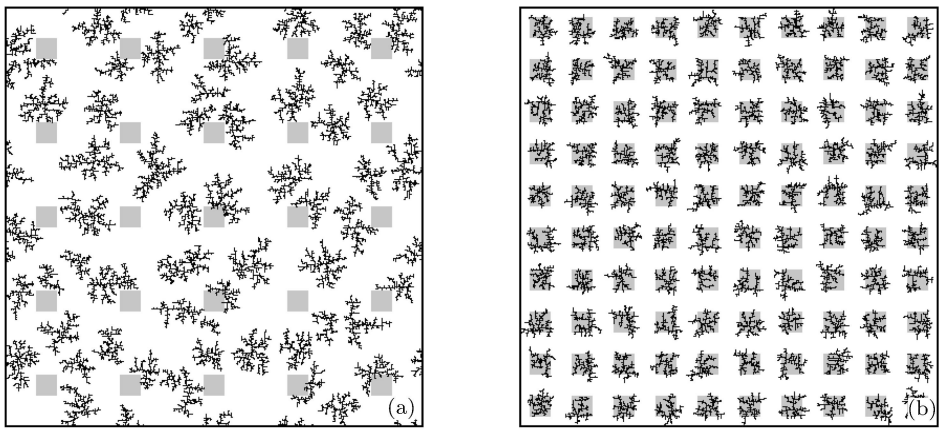


Fig.2. Plots of final morphologies of $E_{\rm AB}(=E_0) \gg E_{\rm BA}(=0)$ (a) and $E_{\rm BA}(=E_0) \gg E_{\rm AB}(=0)$. Parameters used are $L = 400$, $E_0 = 20000$, $E_{\rm A} = E_{\rm B} = 1$, $n = 20000$. Parameters for substrate B are $M = 25$, $L_{\rm B} = 20$ (a) and $M = 100$, $L_{\rm B} = 20$ (b).

We investigated the influence of $E_{\rm AB}$ on the aggregation of particles while keeping $E_{\rm BA} = 0$. Figure 3 presents the dependence of number of clusters N, mean radius of gyration of clusters $\langle R_{\rm g}\rangle$ on the energy $E_{\rm AB}$. The size of cluster is characterized by the radius of gyration

$$R_{\rm g} = \sqrt{\frac{1}{m}\sum_{i=1}^{m} r_i^2}, \qquad (1)$$

where r_i is the distance of the ith particle from the mass centre of the cluster, and m is the number of particles in the cluster. We find that both N and $\langle R_{\rm g}\rangle$ oscillate with $E_{\rm AB}$ after a monotonic increment at small $E_{\rm AB}$. The mean fractal dimension of the cluster has also been calculated. It also vibrates with $E_{\rm AB}$ as N and $\langle R_{\rm g}\rangle$ do. From Fig.3, we find that minimum numbers of cluster occur at special energy values $E_{\rm AB} = 20000, 10000, 6667, 5000, \ldots$, which correspond to the ratios $E_0/E_{\rm AB} = 1, 2, 3, 4, \ldots$. When energies are slightly less than these special values, N can achieve the maximum values.

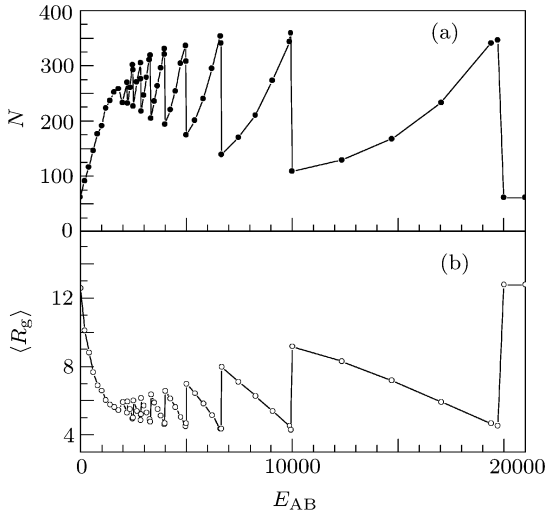


Fig.3. The dependence of the cluster number N (a), and the mean radius of gyration $\langle R_{\rm g}\rangle$ (b) on the energy $E_{\rm AB}$ the particle consumes for moving from substrate A to substrate B, where $L = 400$, $E_0 = 20000$, $E_{\rm A} = E_{\rm B} = 1$, $E_{\rm BA} = 0$, $n = 20000$, $M = 25$, and $L_{\rm B} = 20$.

For $E_{\rm AB}$ slightly less than E_0, some particles may have the possibility to walk into substrate B. If they pass through the AB boundary, then they will consume kinetic energy $E_{\rm AB}$ and soon stop to become new seeds. Figure 4 presents the final morphology for $E_{\rm AB} = 19388$ while $E_0 = 20000$. Here we set $E_{\rm BA} = 0$ so that particles can freely walk out from substrate B. In this case, we find that there are more clusters than at $E_{\rm AB} = E_0$ (Fig.2(a)).

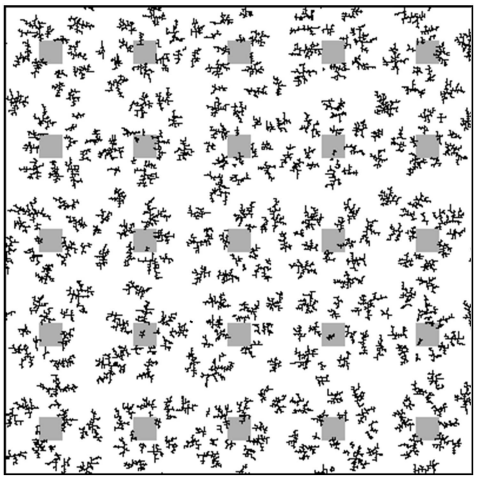


Fig.4. Final morphology at $E_{\rm AB} = 19388$. Parameters: $L = 400$, $E_0 = 20000$, $E_{\rm A} = E_{\rm B} = 1$, $E_{\rm BA} = 0$, $n = 20000$, $M = 25$, and $L_{\rm B} = 20$.

Comparing the final morphology at $E_{\rm AB} = 19388$ (Fig.4) and at $E_{\rm AB} = 20000$ (Fig.2(a)), we find more clusters but smaller in size at $E_{\rm AB} = 19388$. We have also counted the distribution of cluster size for these two cases. Here the cluster size is characterized simply by the particle number m. The results are presented in Fig.5. For the case $E_{\rm AB} = 20000$, particles cannot enter B from A, all particles have energy E_0, and we find a roughly Gaussian distribution of cluster size. However the distribution of size changes in the case $E_{\rm AB} = 19388$. For this case, particles have different diffusion energies in the system. Some particles pass the AB boundary, so they have small diffusion energy $E = E_0 - E_{\rm AB}$, while others have larger diffusion energy $E = E_0$ since they do not cross the AB boundary. This may be the reason for the different distributions of cluster size.

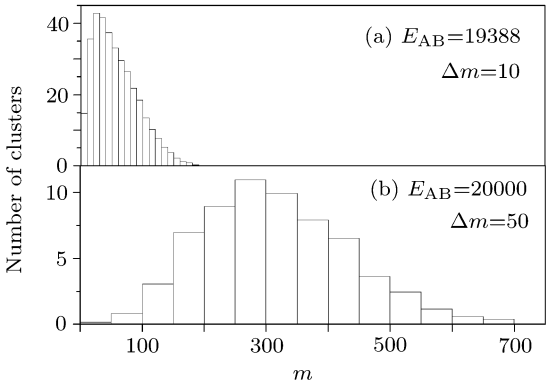


Fig.5. The distributions of the number of clusters against the size of clusters m among $(m - \Delta m, m)$ for $E_{\rm AB} = 19388$ (a) and $E_{\rm AB} = 20000$ (b) respectively. The results are averaged over 50 independent samples. Parameters are $E_0 = 20000$, $n = 20000$, $E_{\rm A} = E_{\rm B} = 1$, $E_{\rm BA} = 0$, $L = 400$, $L_{\rm B} = 20$, and $M = 25$.

For diffusion energy limited aggregation on a homogeneous system where the substrate is of only A or B, the number of clusters N decreases monotonically with the increase of the initial kinetic energy E_0, while $\langle R_g \rangle$ increases monotonically with E_0. However, in the hetero-substrate model, a particle entering substrate B(A) from substrate A(B) needs to consume an additional energy E_{AB} (E_{BA}). Such an additional energy consumed leads to a decrease of energy that a particle can afford in diffusion. It is somewhat equivalent to the decrease of the initial kinetic energy in a homogeneous model. If the E_{AB} (E_{BA}) is small, the energy that a particle should use in diffusion decreases almost smoothly, so the number of clusters N increases monotonically whereas $\langle R_g \rangle$ decreases monotonically (see the beginning of the curves in Fig.3).

With the increase of E_{AB}, the influence of E_{AB} on the diffusion of particles becomes stronger. When E_{AB} is much bigger than E_A and E_B, the diffusion of particles not only depends on the initial kinetic energy E_0, but also on the value of E_{AB}. The effective diffusion energy of a particle is the remaining part of the initial kinetic energy E_0 after subtracting the energy the particle consumes for moving from substrate A to substrate B; and for the case $E_{BA} = 0$ it can be expressed as follows:

$$E_M = E_0 - i_{AB} E_{AB}. \tag{2}$$

Here i_{AB} denotes the times of the particle moving from substrate A to B. The value of i_{AB} can be 0, 1, 2, up to the maximum $E_0/E_{AB} - 1$. So we have the smallest diffusion energy

$$E_{M,min} = E_0 - i_{AB,max} E_{AB}. \tag{3}$$

If $E_{AB} = E_0$, $i_{AB,max}$ must be zero, then no particle can move from A to B. So all the diffusion energy values E_M are the same, i.e., $E_M = E_0$. If $E_0/2 \leq E_{AB} < E_0$, particles have chance to enter B once ($i_{AB,max} = 1$), then the smallest diffusion energy $E_{M,min} = E_0 - E_{AB}$ reaches a maximum at $E_{AB} = E_0/2$. Similarly, we find that the smallest diffusion energy reaches a maximum at

$$E_{AB} = E_0/k_{AB}. \tag{4}$$

At these special values of E_{AB}, we then observe minima in the number of clusters. Figure 6 clearly shows that when E_0/E_{AB} is an integer, there is a minimum of N. Correspondingly, the value of i_{AB} can be 0, 1, 2, up to the maximum $k_{AB} - 1$.

The simulation results indicate that the smallest diffusion energy, which corresponds to the maximum value of i_{AB}, is very important in controlling the cluster number N. If the smallest diffusion energy $E_{M,min}$ reaches a maximum, then the cluster number N is a minimum. Otherwise, if it is small, then N will be large and many small clusters form.

It is very easy to prove that $E_{M,min}$ reaches a local maximum at $E_{AB} = E_0/k_{AB}$ between its two neighbouring values $\dfrac{E_0}{k_{AB}+1}$ and $\dfrac{E_0}{k_{AB}-1}$ for $k_{AB} > 1$. At $E_{AB} = E_0/k_{AB}$, the maximum value of i_{AB} is $k_{AB} - 1$, so the value of $E_{M,min}$ is E_0/k_{AB}. If $E_{AB} = E_0/k_{AB} + \delta$ ($\delta > 0$), then the maximum value of i_{AB} is still $k_{AB} - 1$. In this case we have $E_{M,min} = E_0/k_{AB} - (k_{AB} - 1)\delta$, smaller than E_0/k_{AB}. Similarly, if $E_{AB} = E_0/k_{AB} - \delta$, then we have $E_{M,min} = k_{AB}\delta$, which is also smaller than E_0/k_{AB}. Thus, the smallest diffusion energy reaches its maximum at $E_{AB} = E_0/k_{AB}$, where the cluster number N is a minimum. On the contrary, $E_{M,min} = k_{AB}\delta$ can be very small, then we will find large N at $E_{AB} = E_0/k_{AB} - \delta$, which corresponds to $\dfrac{E_0}{E_{AB}} = k_{AB}\left(1 + \dfrac{\delta}{E_{AB}}\right)$, slightly larger than k_{AB}. It corresponds to a peak as shown in Fig.6.

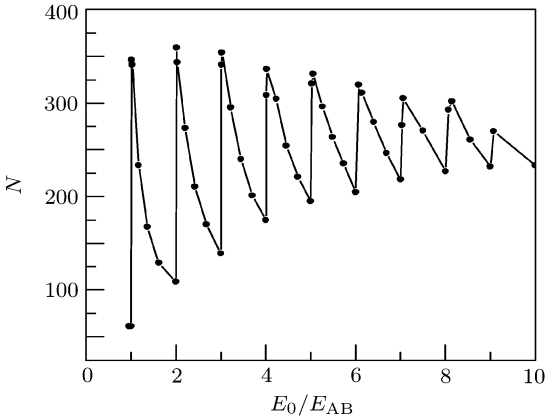


Fig.6. Plot of the number of clusters N versus the ratio E_0/E_{AB}. Data are taken from Fig.3.

When $E_{AB} = E_0/k_{AB} - \delta$ with δ a small positive value, some particles can pass through the AB boundary k_{AB} times for the maximum. Then the smallest diffusion energy $E_0 - k_{AB}E_{AB} = k_{AB}\delta$ can be very small. Therefore, these particles will soon stop after passing AB boundary k_{AB} times and then become extra seeds for clusters. Thus we find a big value of the number of clusters. In simulation a maximum of N is not at $\delta = 1$ but at $\delta = 612$ for $k_{AB} = 1$. The reason is that the number of particles that pass through the AB boundary k_{AB} times, i.e. the number of extra

seeds, increases with δ because particles also consume energy when they diffuse on the A and B substrates. So there is a competition between the smallest diffusion energy and the number of extra seeds, and the maximum of N is reached at a special value of $E_{\rm AB}$.

A particle stops if it uses up all of its energy or contacts with other seeds or clusters. During the simulation, we have recorded the diffusion length for each particle. We counted the distribution of particle number versus the diffusion length and averaged it for 100 samples. The diffusion length is the total steps of particle moving on the lattice. The results for $E_{\rm AB} = 20000$ where N is minimum and for $E_{\rm AB} = 19388$ when N is maximum are presented in Fig.7. We find that more particles can move a longer distance at $E_{\rm AB} = 20000$. There are about 64 particles moving 20000 steps. The value 64 is slightly larger than the final cluster number $N = 61$ in Fig.3(a) because some adjacent clusters may be reconnected with other particles to form one big cluster. Therefore, these 64 particles can be regarded as isolated seeds in the system, while for $E_{\rm AB} = 19388$, the number of particles that can move 20000 steps is 28. Besides, there is a peak for a diffusion length of $N_{\rm step}$ near $E_0 - E_{\rm AB} = 612$. This means that many particles can only move 612 steps, indicating that these particles may pass the AB boundary and they may become seeds quickly. The height of the bar at the peak value is about 316. Then the total seeds are about 344. It is also very close to the value of cluster number $N = 346$ at $E_{\rm AB} = 19388$ in Fig.3(a).

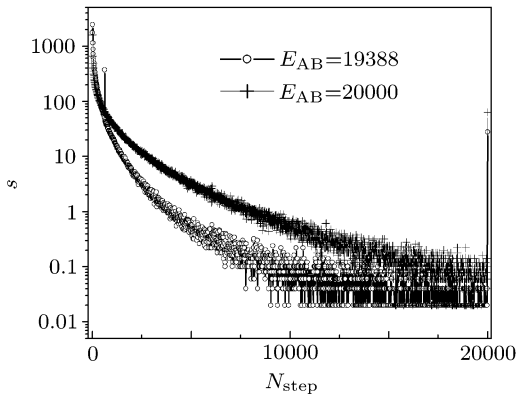


Fig.7. Distributions of particle number s versus diffusion length $N_{\rm step}$ for two boundary energies $E_{\rm AB} = 20000$ and 19388. Simulation parameters are the same as that of Fig.3. In counting the values of distributions, the interval of diffusion step is taken to be 10. 1000 samples are used for statistics.

A similar phenomenon is observed when we change the initial kinetic energy E_0 while $E_{\rm AB}$ is kept a constant. Figure 8 presents the variation of the number of clusters with E_0. We find that N reaches its minimum at $E_0 = kE_{\rm AB}$ (or $E_{\rm AB} = E_0/k$) and reaches its maximum at $E_0 = kE_{\rm AB} + \delta'$ (or $E_{\rm AB} = E_0/k - \delta$). For this case, the period of the vibration is equal to $E_{\rm AB}$.

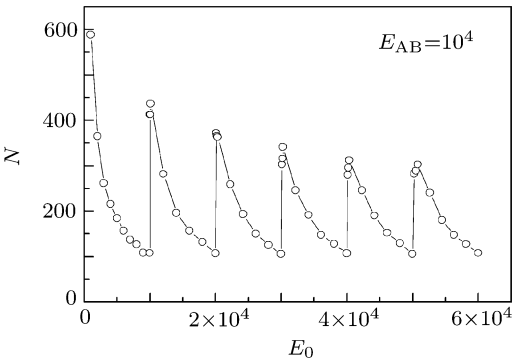


Fig.8. The dependence of the number of cluster N on the initial kinetic energy E_0 for $E_{\rm AB} = 10000$. Parameters are $E_0 = 20000$, $n = 20000$, $E_{\rm A} = E_{\rm B} = 1$, $E_{\rm BA} = 0$, $L = 400$, $L_{\rm B} = 20$, and $M = 25$.

We have also investigated the influence of $E_{\rm BA}$ on the aggregation of particles. Simulations are carried out for a system with following parameters: $E_0 = 20000$, $n = 20000$, $L = 400$, $E_{\rm A} = E_{\rm B} = 1$, $M = 25$ and $L_{\rm B} = 20$, while $E_{\rm AB}$ and $E_{\rm BA}$ are two variables. Figure 9 presents the variation of the cluster number N with $E_{\rm AB}$, while $E_{\rm BA}$ is a constant. When $E_{\rm BA} \neq 0$, the situation becomes a little complicated. The remaining energy

$$E_{\rm M} = E_0 - i_{\rm AB}E_{\rm AB} - i_{\rm BA}E_{\rm BA} \tag{5}$$

for a particle passing through the boundaries AB and BA $i_{\rm AB}$ and $i_{\rm BA}$ times, respectively. For the case $E_{\rm BA} \ll E_0$, we find that there are many minima of cluster number N. The places of these minima are summarized as

$$E_{\rm AB} = \frac{E_0 - k_{\rm BA}E_{\rm BA}}{k_{\rm AB}} \tag{6}$$

with $k_{\rm AB}$ and $k_{\rm BA}$ two integers. We define main minima where $k_{\rm AB} = 1, 2, \ldots$, while $k_{\rm BA}$ is restricted to $k_{\rm BA} = k_{\rm AB} - 1$. Besides the main minima, we find that there are two local minima between two neighbour main minima. For the two local minima, the value of $k_{\rm BA}$ can only be taken as $k_{\rm BA} = k_{\rm AB}$ and $k_{\rm BA} = k_{\rm AB} + 1$. For example, if we adopt $E_0 = 20000$, $E_{\rm BA} = 500$ as used for Fig.9(a), we then have the first three main minima at $E_{\rm AB} = 20000$, 9750 and 6333, the first two local minima at $E_{\rm AB} = 19500, 19000$, and the second two local minima at $E_{\rm AB} = 9500$, 9250. These locations are indicated in Fig.9(a) as (a), (b),

(c) for three main minima, and (a1), (a2), (b1), and (b2) for four local minima.

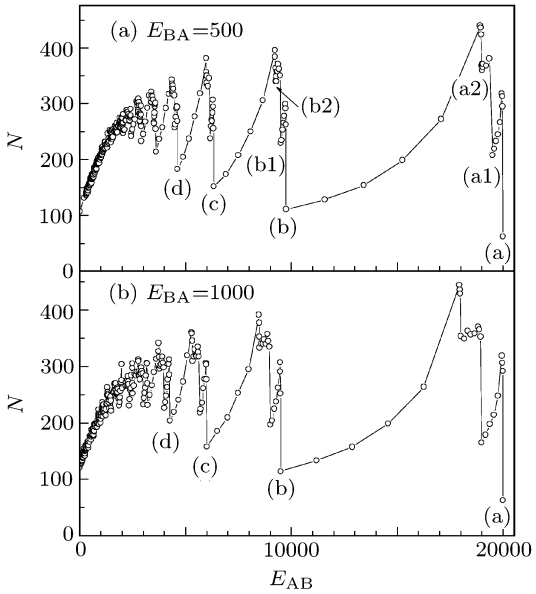


Fig.9. The dependence of cluster number N on energy E_{AB} that the particle consumes moving from substrate A to substrate B while the energy from B to A is kept constant $E_{BA} = 500$ (a) and $E_{BA} = 1000$ (b). Other parameters are $E_0 = 20000$, $n = 20000$, $E_A = E_B = 1$, $L = 400$, $L_B = 20$, and $M = 25$.

Particles in a system can or cannot pass through its boundaries. Figure 10 gives routines for a particle passing through boundaries at maximum times for $E_{AB} > E_{BA}$. With these routines, a particle has a minimum energy for diffusion. The minimum diffusion energy controls the final morphology of clusters as for the case $E_{BA} = 0$. At the special values of E_{AB} given in Eq.(6), we can also prove that the minimum energy for diffusion is a local maximum. Then the cluster number N is minimum at these special values of E_{AB}. When $E_{AB} < E_{BA}$, we could just reverse these routines. For a specific case $E_{AB} = E_{BA} = E_0/2$, Fig.10(b) with $k_{AB} = k_{BA} = 1$ is the only possibility.

Figure 11 presents four morphologies at two main minima $E_{AB} = 20000$ and 9750, one local minimum $E_{AB} = 19500$, and a maximum $E_{AB} = 19940$. At the main minimum $E_{AB} = 20000$, particles can only move out from substrate B, as shown in Fig.10(a). Therefore, we find that almost all particles are in the substrate A, and they form large clusters since they have large diffusion energy. A similar situation is seen at another main minimum $E_{AB} = 9750$, where particles can pass AB and BA boundaries and stay on the substrate A as shown in Fig.10(d). Then we find that most particles are in substrate A as shown in Figs.11(a) and 11(b).

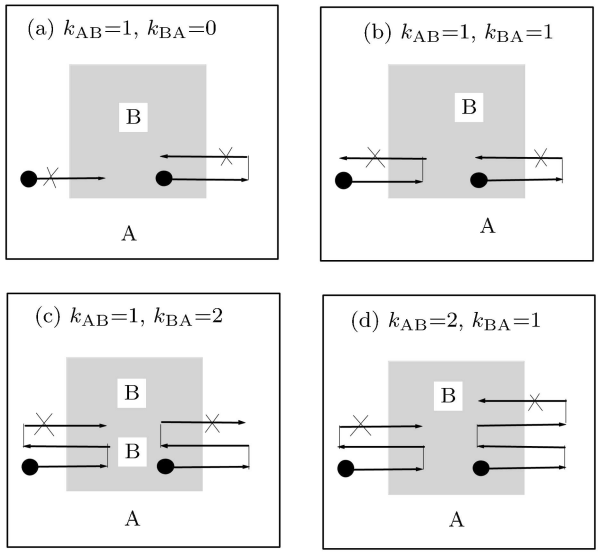
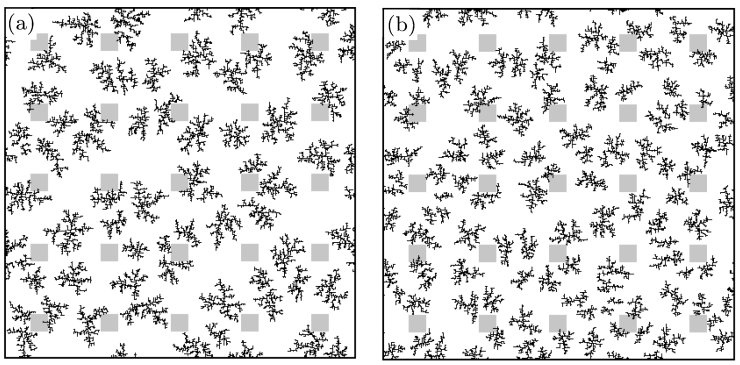


Fig.10. Schematic diagram of routines for a particle moving through boundaries for 4 cases with different k_{AB} and k_{BA}. With these routines, a particle has a minimum energy for diffusion. The boundary energy E_{BA} is constant and E_{AB} is given by Eq.(6). The grey square represents substrate B, while the remainder represents substrate A (white). Particles are represented by solid circles. An arrow without a cross means an allowed path for particles, while the one with a cross shows a forbidden path for particles.



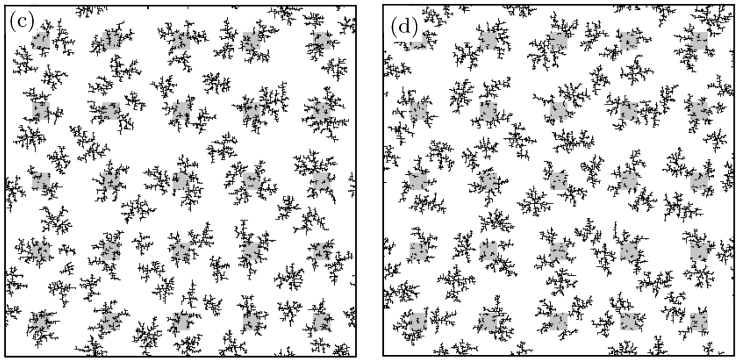


Fig.11. Final morphologies at different $E_{\rm AB} = 20000$ (a), 9750 (b), 19500 (c) and 19940 (d). Other parameters are $E_0 = 20000$, $n = 20000$, $E_{\rm A} = E_{\rm B} = 1$, $L = 400$, $L_{\rm B} = 20$, $M = 25$, and $E_{\rm BA} = 500$.

At local minimum $E_{\rm AB} = 19500$, however, particles which pass the AB boundary and enter substrate B cannot diffuse out of it and vice versa, as shown in Fig.10(c). Thus there are a lot of particles in substrate B as shown in Fig.11(c). At $E_{\rm AB} = 19940$, particles have smaller remaining energy than at $E_{\rm AB} = 19500$, so we find more small clusters in substrate B for $E_{\rm AB} = 19940$.

Equation (6) is also valid for large $E_{\rm BA}$ only if $E_0 - k_{\rm BA}E_{\rm BA}$ is positive. The largest $E_{\rm BA}$ is $E_0/2$ due to the symmetry of the system. We find that Eq.(6) is still valid for $E_{\rm BA} = E_0/2$. The result for $E_{\rm BA} = E_0/2$ is presented in Fig.12 where $E_0 = 20000$. We can observe four minima at $E_{\rm AB} = 20000$, 10000, 5000, and 0. From the routines shown in Fig.10, one can see that $E_{\rm AB} = 20000$ and 5000 corresponds to two main minima with $k_{\rm AB} = 1$, $k_{\rm BA} = 0$ and $k_{\rm AB} = 2$, $k_{\rm BA} = 1$, respectively. While $E_{\rm AB} = 10000$ and 0 corresponds to two local minima with $k_{\rm AB} = 1$, $k_{\rm BA} = 1$ and $k_{\rm AB} = 1$, $k_{\rm BA} = 2$, respectively.

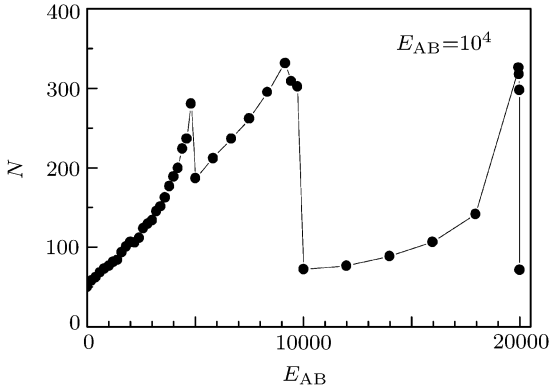


Fig.12. The dependence of the cluster number N on the energy $E_{\rm AB}$ when $E_{\rm BA} = 10000$. Other parameters are the same as in Fig.9.

4. Conclusion

We have proposed a model to study the aggregation of particles on a hetero-substrate which may be made by using two different materials or two materials with different physical properties. The model is based on the aggregation of metallic atoms on molten glass surface where a lot of impurity regions were found. The hetero-substrate in our model is composed of two substrates A and B with finite surface barriers $E_{\rm AB}$ and $E_{\rm BA}$ between the AB and BA boundaries, respectively. With the DELA model, we discover a law that governs the aggregation properties. The law can explain the dependence of the number of clusters and mean radius of gyration on the surface barriers $E_{\rm AB}$ and $E_{\rm BA}$. For the case of $E_{\rm BA}$ being a constant, we observe a series of main minima and two local minima between two neighbouring main minima. The positions of these minima can be expressed as $E_{\rm AB} = \dfrac{E_0 - k_{\rm BA}E_{\rm BA}}{k_{\rm AB}}$ with $k_{\rm AB}$ and $k_{\rm BA}$ being two integers. For the main minima, we have $k_{\rm AB} = 1, 2, \ldots,$ while $k_{\rm BA}$ is restricted to $k_{\rm BA} = k_{\rm AB} - 1$ while for the two local minima, $k_{\rm BA}$ can only be $k_{\rm BA} = k_{\rm AB}$ and $k_{\rm BA} = k_{\rm AB} + 1$. However, the number of local minima may decrease since $E_0 - k_{\rm BA}E_{\rm BA}$ is restricted to positive values. Moreover, for $E_{\rm BA} = 0$ only main minima are found at $E_{\rm AB} = E_0/k_{\rm AB}$. Different aggregation morphologies have been observed and the results explained.

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