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One-dimensional crystal growth model on a square lattice substrate

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ABSTRACT

A one-dimensional crystal growth model along the preferential growth direction is established. The simulation model is performed on a square lattice substrate. First, particles are deposited homogeneously and, as a result, each of the lattice sites is occupied by one particle. In the subsequent stage, N nuclei are selected randomly on the substrate, then the growth process starts by adsorbing the surrounding particles along the preferential growth directions of the crystals. Finally, various one-dimensional crystals with different length and width form. The simulation results are in good agreement with the experimental findings.

1. Introduction

The growth of various nanostructures, such as ramified aggregates, nanorings, nanowires etc., has attracted much attention in recent decades owing to its theoretical importance and applicable purposes [1–6]. If the experimental conditions are carefully selected, one-dimensional nanostructures may be fabricated on crystal substrates since the deposition atoms may diffuse on the substrates along the crystal surface directions [7]. Generally, it is difficult to produce orientational nanostructures on isotropic surfaces.

Liquid surfaces exhibit isotropic characteristics which may be used to fabricate various nanostructures without specific orientations [2,3,8]. For example, after the metallic atoms were deposited on silicone oil surfaces by thermal evaporation method [2,9–12], they diffuse on the liquid surfaces by Brownian motion and the mean square diffusion displacement $\langle \Delta r^2 \rangle$ is given by $\langle \Delta r^2 \rangle = 4D\Delta t$, where D is the diffusion coefficient and Δt is the time [13,14]. Finally, branched metallic aggregates with polycrystal microstructure form. This growth mechanism can be well explained by the two-stage growth model [2]. The following research showed that organic crystals with branched morphology may also be fabricated on liquid surfaces [3,8].

Recently, one-dimensional zinc crystals were fabricated successfully on silicone oil surfaces by Lu et al. [15], which provides a new method to grow one-dimensional metallic nanostructures on liquid surfaces. It is well known that, just as beryllium, magnesium and cadmium crystals, zinc crystal exhibits the hexagonal structure and possesses preferential growth directions (direction [002], for instance) [16]. TEM measurement confirmed that the Zn crystals mainly grow along the preferential growth directions [15]. Therefore, it is suggested that one-dimensional crystals may also grow on various isotropic surfaces if the crystals possess preferential growth directions.

In this paper, in order to explain the growth mechanism of one-dimensional crystals (namely, crystal rods) on isotropic substrates, a computer simulation model is established, in which the significant crystal growth characteristic with a preferential growth direction is used. The simulation results are in good agreement with the experimental observations [15].

2. Model description

The computer simulation is performed on a square lattice substrate with periodic boundary conditions, where the lattice constant $a_0 = 1$ and the size of the substrate is $S = 500 \times 500$. The growth model is defined as follows:

1) Particles are deposited on the square lattice substrate homogeneously, as a result, each of the lattice sites is occupied by one particle.

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2) A nucleation site is randomly picked and all the particles in the area $l \times l$ around the site aggregate and form a crystal seed with the size of $W \times W$, where size l may be chosen from all the even numbers (since the seed is located in the center of the area $l \times l$) between 1 and $l_{\max}$ randomly and $W = \sqrt{l}$. Repeat this process until the total number of the seeds reaches a preset value N. If the area $l \times l$ of a new seed overlaps with that of others, delete this nucleation site.
3) The preferential growth direction for each seed may be horizontal (left and right) or vertical (up and down), which is selected by the computer randomly and then fixed in the simulation.
4) In the subsequent growth process, a seed or a crystal rod is randomly picked and one of the two nearest sites along the preferential growth direction is also randomly selected as the growing tip. The particles in the area $l \times l$ around the tip aggregate and the crystal rod grows in this direction with length a_0 and width W. The tip will stop growing if the area $l \times l$ around it meets that of others.
5) Repeat step (4) above until all the crystal rods stop growing.

For the sake of simplicity, we suppose that the crystal rods in the model above exhibit the simple cubic lattice structure and the cross section of the rods is square. Based on the conservation law of matter, we have

$$a_0 l \Delta L = W^2 \Delta L, \tag{1}$$

where ΔL is the increment of the rod length L. Therefore, $W = \sqrt{l}$ (as shown in the second point of the model above). For each rod, since l is selected randomly from the even numbers between 1 and $l_{\max}$ and then fixed in the growth process, therefore W remains unchanged during the growth of the rod.

We also suppose that, when the particles aggregate, they may continue to diffuse due to the interaction among them until the lowest energy of the system is achieved. When a particle meets with a crystal rod, it may diffuse along the rod surface until the lowest surface energy is obtained. In other words, the growth of the straight crystal rods with parallel edges along the preferential growth directions results from the minimal energy principle [15].

Besides, based on the experimental results [15], we set $N =$ 50–400 and $l_{\max} = 200$ in the following simulation.

3. Results and discussion

The typical simulation images are shown in Fig. 1, where crystal rods with different widths, lengths and orientations are irregularly distributed on the substrate. Since both the nucleation sites and the aggregation size l are selected randomly by the computer, it is quite reasonable that the lengths and widths of the rods are nonuniform. From the experimental point of view, the rods with long length L, small width W and large ratio $\delta \equiv L/W$ are generally expected. In our simulation, if $N = 50$, the length of the longest rod is $L_{\max} = 494$; the width of the most fine rod is $W_{\max} = 1.41$; the maximum value of δ is $\delta_{\max} \equiv (L/W)_{\max} = 285$. If $N = 150$, then $L_{\max} = 198$, $W_{\max} = 1.41$, $\delta_{\max} = 140$. Therefore, the morphologies and distributions of the rods shown in Fig. 1 are quite similar with that observed in experiment [15].

In order to produce very thin rods (or wires) with very large ratio δ, the seed number N should not be too large and the overlap phenomenon among the rods should be avoided. Therefore, Fig. 1 shows the basic idea of the growth mechanism and gives the information to control the morphologies of the rods in experiment.

The simulation was repeated more than one hundred times and then more than 25 000 rod samples could be taken into account. The length and width distributions of the crystal rods are shown in Fig. 2, in which the solid lines are the fits to the simulation data. It is noted that both the length and width distributions are in concordance with the lognormal distribution. The most probable length and width ranges are 10–20 and 1.6–2.8, respectively. Similar asymmetric distributions shown in Fig. 2 are also observed in experiment [15,17]. In fact, all the simulation results are relative. If we change the units of the length L, width W and Count in Fig. 2, then the obtained length and width distributions may be in good agreement with the experimental observations [15].

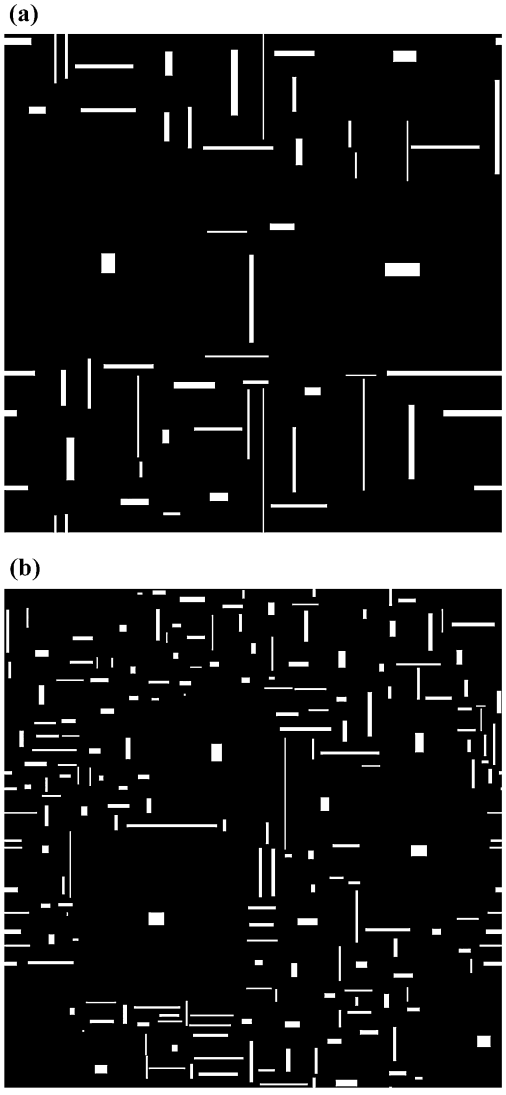

Fig. 1. Images of the simulation results: (a) $N = 50$, and (b) $N = 200$.

The statistical descriptions for the dependences between the rod sizes and N are shown in Figs. 3(a) and 3(c), in which the peaks of the length and width distributions increase and approach left as N increases. This phenomenon indicates that the size dispersion degree may be reduced by increasing the seed number N.

The average length $\langle L \rangle$ and width $\langle W \rangle$ of the rods were measured for more than 25 000 rods in our simulation and both drop quickly as N increases. We find that $\overline{\delta} \equiv \frac{\langle L \rangle}{\langle W \rangle}$ decreases from 10.5 to 5.4 when N increases from 50 to 400, indicating the average morphology evolution of the rods as N increases. Experimentally, N is related to the deposition rate, nominal thickness, substrate temperature, diffusion coefficient, etc. Therefore, the morphology of the crystals may be controlled in experiment by selecting experimental conditions.