Modelling of Columnar Growth in Continuum Ballistic Deposition

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The evolution of the surface morphology during the growth and deposition of the film has been a subject of intense interest for the last few years [1]. As a result, a variety of simple models have been studied. One example is the ballistic deposition model that corresponds to the irreversible sticking of particles to the growing film under the assumption that the mean free length of the particles is larger than the film morphology size.

Previous theoretical and computational studies of the ballistic deposition have involved computer simulations of the aggregation of discrete particles [1] and the use of continuum stochastic partial differential equations [2,3]. However, there are some defects in these models: The discrete description does not incorporate surface diffusion in a natural way, and the differential equation approach is limited to the no-overhang interface approximation and does not accommodate nonlocal effects. Furthermore, more realistic molecular dynamics simulations [4] are limited to small sizes of the system. To overcome these faults, we propose a new continuum model to describe the growth dynamics of the film surface in continuum ballistic deposition.

Our model involves two fields f and g, and is described by the equations

$$\begin{aligned} \frac{\partial}{\partial t} f(\mathsf{r}, t) &= \nabla^2(-f + f^3 - a\nabla^2 f) \\ &\quad + B(\nabla f)^2 g(\mathsf{r}, t) \qquad (1) \\ \frac{\partial}{\partial t} g(\mathsf{r}, t) &= \nabla(D\nabla g - Ag) \\ &\quad - B(\nabla f)^2 g(\mathsf{r}, t) \qquad (2) \end{aligned}$$

Our phenomonological model is designed to satisfy the simple physical requirements described below. Setting $g \equiv 0$ in the model, we recover the familiar equation for the conserved order parameter field f in phase separating systems having two equilibrium phases $f = 1$(growing film) and $f = -1$ (vacuum) [5]. The interface or film surface is defined by $f = 0$ with the interfacial width $\sqrt{a}$. This description allows for arbitrary interface topologies. The g field represents the local density of the incoming particles toward the interface. When $f \equiv 0$, eq.(2) for the g field is the diffusion constant D in the presence of an external force A ($= -A\hat{z}$ in the present simulations). Finally, the B terms provide the coupling between the f and g fields. The B terms represent the mechanism such that the growth of the f field occurs at the expense of the g field in the vicinity of the interface ($(\nabla f)^2 \sim 0$ far from the interface).

To discuss the morphological evolution of the growing film surface in ballistic depositions, we have solved numerically the above equations (1) and (2) in two dimensions, starting from proper initial conditions and boundary conditions [5]. Typical simulation results of the time evolution of the growing film surface morphology are shown in Figs.1-3 for three different values of B. In these figures at large times, we observe the flat surface for small value of B, regularly arranged columnar pattern for intermediate B, and irregularly branched columns for large B. These results are in qualitatively agreement with recent experimental date [6].

The present model might provide a unified picture of several growth processes of the film surface morphology. Further simulation results and analytic treatment of the model will be discussed in the conference, as well as three dimensional results.

References

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