**Controlling nanostructures: A model with deposition, diffusion and aggregation**

SIR - Röder et al. report nanometre-scale structures built by deposition of diffusing particles that aggregate on surfaces [1]. We report a computer model that mimics the same process, and produces morphologies that remarkably resemble the experimental structures. The model is defined as follows:

(a) *Deposition.* Particles are deposited at randomly-chosen positions of the surface at a flux $F$ per lattice site per unit time.

(b) *Diffusion.* A cluster of connected particles is chosen at random and moved North, East, South or West by one lattice constant with a probability proportional to its mobility, which is given by $D_s = D_1 s^{-\gamma}$, where $s$ is the number of particles in the cluster, $D_1$ is the diffusion constant of the monomers and $\gamma$ characterizes how the mobility of a cluster depends on its size.

(c) *Aggregation.* If two particles come to occupy neighboring sites, they stick irreversibly.

The model can be tested by explicit comparison with the experimental data of [1], since there are no free parameters provided we introduce the experimental values for the flux and the diffusion constant. The diffusion constant of the monomers is given by $D_1(T) = D_0 \exp(-E_d/kT)$ with $E_d = 0.14eV$ [1], and $D_0 = 5 \times 10^{11}$ [2]. Using the experimental values of the fluxes, we find $F/D_1 = 10^3$ corresponds to Fig. 1a of [1], and $F/D_1 = 10^{-10}$ to Fig. 1d. Figs.1a,b show results of the model with these flux values, and we note that the morphologies compare well with Figs. 1a and 1d of [1].

In general, the model allows one to distinguish the effects of deposition, diffusion and aggregation. We find that tuning the relative strength of, e.g., deposition and diffusion, generates a rich range of morphologies—including diffusion limited aggregation, cluster-cluster aggregation, and percolation [3]. The length and time scales characterizing these morphologies depend on experimentally-controllable parameters like deposition flux, and diffusion constant, raising the possibility that the model can be used for a controlled design

of nonostructure morphologies. Indeed, the model makes specific predictions, for example that the typical size of the DLA-like structures scales as $(F/D_1)^{1/4}$.

The model may be useful in many situations where diffusion occurs in the presence of continuous deposition. The model was originally motivated by thin film deposition experiments in which not *isolated atoms* but rather *aggregates* made up of compact spherical "molecules", ≈5 nm diameter containing ≈2000 atoms are deposited on a surface [4]. The morphologies of Figs.1a,b also resemble experimental images obtained by such LECBD experiments on substrates maintained at low temperatures (compare Fig. 1b to Fig.3 of Ref.4).

Pablo Jensen, Albert-László Barabási, Hernán Larralde, Shlomo Havlin & H.Eugene Stanley

Center for Polymer Studies and Physics Department, Boston University, Boston, MA 02215

1. Röder, H. Hahn, E., Brune, H., Bucher, J.-P., & Kern, K. *Nature* **366**, 141-143 (1993).
2. Venables, J.A., Spiller, G.D.T. & Hanbücken, M., *Rep.Prog.Phys.* **47**, 399-459 (1984).
3. Vicsek, T. *Fractal Growth Phenomena, 2nd Ed.* (World, Singapore, 1992)
4. Jensen, P., Melinon, P., Hoareau, A., J. X. Hu, B. Cabaud, M. Treilleux, E. Bernstein & D. Guillot, *Physica A* **185**, 104-110 (1992)

Fig.1: Morphologies obtained in the present model for two different values of flux $F$, diffusion constant $D_1$, and total surface coverage all chosen to correspond to the experimental parameters used in obtaining the data shown in Figs. 1a and 1d of Ref.1. (a) $F/D_1 = 10^3$, and total coverage of 0.012 (b) $F/D_1 = 10^{-10}$, and total coverage of 0.12. The simulation lattice had $200 \times 200$ sites; the portion shown here corresponds to Figs. 1a and 1d of Ref.1, which are also a portion of the total experimental system. We set $\gamma = 10$ (larger clusters rarely move—J.P. Bucher, private communication).