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MONTE-CARLO SIMULATION OF SURFACE GROWTH

Final Report

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FINAL REPORT

We have carried out simulations using various methods on models of epitaxial growth. We have investigated both homoepitaxial as well as heteroepitaxial growth. We have studied the effects of evaporation, island coarsening, strain due to lattice mismatch, three-dimensional islands submonolayer growth and self-organization in quantum dot superlattices. The results of our investigations are of significance to the understanding of material properties at the nanoscale.

A. PUBLICATIONS

Seven paper have been published and three others have been submitted for publication:

[1] *Renormalization group study of Mullins' equation for molecular beam epitaxy with conserved noise*, Pui-Man Lam and Diola Bagayoko, Physica **A250**, 495 (1998)

The dynamics of driven interfaces under conserved noise in a continuum model of growth by a molecular beam has been studied by means of the Nozieres-Gallet dynamic renormalization group technique, using the results of Sun and Plischke for the case of non-conserved noise. Relaxation of the growing film id due to both surface tension and surface diffusion. In (1+1) dimensions, four growth regimes have been found. None of these are pure diffusive. One of these fixed points has negative surface tension and is stable with respect to renormalization group flow. This is an unstable growth state in which the creation of large slopes in the interface configuration is expected. In (2+1) dimensions, seven growth regimes have been found, in which three are purely diffusive. There is also one fixed point with a negative surface tension. However, this fixed point is unstable with respective to renormalization group flow, and is therefore expected to crossover into the other growth regimes at large system size and long times.

[2] *Effects of randomness and spatially dependent relaxation on sandpile models*, Pui-Man Lam, Isiaka Akanbi and David E. Newman, Physica **A253**, 307 (1998)

We investigate two types of randomness in the relaxation of sandpile models when the slope at some point becomes over critical. In one type of randomness, the number of particles n_f, falling to its nearest neighbors in the resulting relaxation, is not constant but random, even though an equal number fall in each direction. We find that this kind of randomness does not change the universality class of the models. Another type of randomness is introduced by having all n_f particles to fall in one single direction, but with the direction chosen randomly. We find that this type of randomness has a strong effect on the universality of the models.

[3] *Effects of monomer evaporation in the Clarke-Vvedinsky model of submonolayer growth*, Pui-Man Lam, Rahman Tashakkori and Ke Yu, Phys. Rev. **B56**, 4893 (1997)

We investigate the Clarke-Vvedensky model in thin film growth, taking into account the possible evaporation of particles deposited in the surface. This is a reversible growth model in which surface atoms in an island can break loose with a probability proportional to $\exp(-nE_N/k_BT)$, where n is the number of lateral bonds and E_N is a fixed pair bond energy. We find that the presence of evaporation can dramatically affect the growth kinetics of the film and give rise to regimes characterized by different island size distributions.

[4] *Monte-Carlo simulation of coarsening in a model of submonolayer epitaxial growth*, Pui-Man Lam, Diola Bagayoko and Xiao-Yang Hu, Surf. Sci. **429**, 161 (1999)

We investigate the effect of coarsening in the Clarke-Vvedensky model of thin film growth, primarily as a model of statistical physics far from equilibrium. We deposit adatoms on the substrate until a fixed coverage is reached. We then stop the deposition and measure the subsequent change in the distribution of the island sizes. We find that for large flux, coarsening in this model is consistent with the Lifshitz-Slyozov law $\xi \sim t^{1/3}$, where ξ is the characteristic linear dimension and t is the time in the coarsening process. We have also calculated the stationary states of the island size distributions at long times and find that these distribution functions are independent of initial conditions. They obey scaling with the universal scaling function agreeing with that obtained by Kandel using the Smoluchowsky equation in a cluster coalescence model.

[5] *Monte-Carlo investigation of island growth in strained layers*, Sovirith Tan and Pui-Man Lam, Phys. Rev. **B59** 5871 (1999)

A treatment of kinetic Monte-Carlo method is devised that incorporates strain effects in a direct and natural way. The submonolayer growth ($\theta<0.3$) of islands, in the cases of negative misfits (-10% and –32%) and of positive misfits (+10%, +20% and +32%), is considered. The case of negative misfits leads to smaller islands, whereas the case of positive misfits leads to larger islands. It is inferred, from these drastic effects of strain on heteroepitaxial nucleation, that the adatoms at low coverage ($\theta<0.3$), is subject, during the growth regime ($0.05<\theta<0.2$), to a bias force generated by compressive or tensile strain at interface, which promotes detachment or attachment from islands, respectively.

[6] *Monte-Carlo simulation of three-dimensional islands*, Sovirith Tan and Pui-Man Lam, Phys. Rev. **B60**, 8314 (1999)

The usual kinetic Monte-Carlo method is adapted, to treat off-lattice problems of multilayer growth (coverage $\theta>1$) by molecular-beam epitaxy. This method takes into account the Schwoebel barrier, which comes out as a result of the choice of the potential interaction between the atoms. This method allows a free choice of the lattice mismatch, temperature, deposition flux rate, and interfacial energies. A particular choice of these parameters leads to three-dimensional (3D) (Volmer-Weber) growth mode, whereas another choice of these parameters leads to 2D-3D growth mode (Stranski-Krastanov). The 3D islands seem to obey scaling only approximately. Using this method, the surface stress inside a substrate and a (pyramidal) coherent 3D island is computed. Strong relaxation appears, not only at the edges of the 3D island (which is expected), but also in the proximity of the edges, and inside the 3D island. These particular sites inside the 3D island are located just beneath a step site of the upper layer. Strain-induced modulation of

layers is thermally activated, so the steps could act as defects and nucleation sites for propagating roughness, in agreement with some theories and experimental facts.

[7] *Extremal-point densities of interface fluctuations in a quenched random medium*, Pui-Man Lam and Sovirith Tan, Phys. Rev. **E62**, 6247 (2000)

We give a number of exact, analytical results for the stochastic dynamics of the density of local extrema (minima and maxima) of linear Langevin equations and solid-on-solid lattice growth models driven by spatially quenched random noise. Such models can describe nonequilibrium surface fluctuations in a spatially quenched random medium, diffusion in a random catalytic environment, and polymers in a random medium. In spite of the nonuniversal character for the quantities studied, their behavior against the variation of the microscopic length scale can present generic features, characteristic of the macroscopic observables of the system.

[8] *A kinetic Monte-Carlo model of self-organized quantum dots superlattices*, Pui-Man Lam and Sovirith Tan, submitted

We study a model of self-organized growth of quantum dots superlattices using spacer layers of Si with Ge islands buried inside. At each new spacer layer, Ge atoms are deposited on the new Si surface with a flux F. These atoms diffuse on the Si surface with diffusion constant D. But the diffusion of these Ge atoms are biased due to the strain field of the buried Ge islands in the previous layer. When these diffusing atoms meet one another they nucleate into islands which then grow by capturing other adatoms. When the Ge coverage reaches a fixed value θ, these islands are buried under Si up to a thickness L to complete a new spacer layer. We find that after many successive spacer layers, both the island size distribution and the island spacing become more uniform. However, the island spacing is controlled by the ratio D/F rather than by the spacer thickness L. Also the island density $\rho \sim (D/F)^{1/4}$, as in the case without strain, but with a different prefactor.

[9] *Monte-Carlo investigation of vertical correlations in self-organized multilayer growth of islands*, Sovirith Tan, Pui-Man Lam and J.C.S. Levy, submitted

The usual kinetic Monte-Carlo method, adapted to treat off-lattice problems, is used to investigate the experimental observation of the vertical self-organization of buried islands, grown in heteroepitaxial multilayers films. It is found that, during the early stage of island nucleation and growth (before Otswald ripening), the adatoms diffuse to preferential sites, just above the centers of the buried islands, resulting in the vertical replication of the islands. Starting from an ordered island array, this ordered configuration is reproduced during the subsequent growth of the multilayer. Starting from a 'quasi-order' island array, where a few islands are larger than the others, it is found that the system relaxes quickly within two bilayers towards the common island size. The distribution curve of the vertical correlation is reported. The map of the stress inside a spacer layer is calculated by means of molecular dynamics models. All these results confirm the model of the island-induced strain field resulting in the directed diffusion of adatoms above the buried islands. All these results come out naturally from the off-lattice model described above.

[10] *Excluded volume effects in gene stretching*, Pui-Man Lam, submitted

We investigate the effects of excluded volume on the stretching of a single DNA in solution. We find that for small force F, the extension h is not linear in F but proportion to F^{γ}, with $\gamma=(1-\nu)/\nu$, where ν is the well-known universal correlation length exponent. A freely joint chain model with the segment length chosen to reproduce the small extension behavior gives excellent fit to the experimental data of λ-Phage DNA over the whole experimental range. We show that excluded volume effects are stronger two dimensions and also derive results in two dimensions which are different from the three dimensional results. This suggest experiments to be performed in these lower dimensions.

B. GRADUATE STUDENTS

Three graduate students finished their master degree thesis based on research in this project. Ke Yu based her 1998 master thesis on publication [3] above. She is now working for Microsoft in Seattle in soft-ware development. Xiao-Yang Hu based his 1999 master thesis on publication [4]. He is now working for AT&T in Seattle in program development. Isiaka Akanbi based his 1999 master thesis on publication [2]. He is now working as electrical engineering for GE in Chicago.

C. BUDGET

The budget has now been extended at no cost to September 14, 2001.