A CELLULAR AUTOMATON FOR MODELLING EVOLUTION OF HETEROEPITAXIAL SYSTEMS

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Summary An algorithm is presented for the implementation of surface and bulk diffusion within a cellular automaton. Relaxation of the elastic strain in heteroepitaxial systems via morphological change and interdiffusion is investigated.

INTRODUCTION

The large elastic strain energy present in epitaxial heterogeneous thin film systems due to elastic mismatch acts to destabilize the growth of a flat planar film. This can lead to the development of self-organised clusters of atoms which have many potential microelectronic and optoelectronic applications. The electronic properties of these islands (clusters) is highly dependent on their internal strain state. The mismatch strain originates from the compositional differences within these multi-component systems. During deposition these structures can evolve to reduce the compositional variations by alloying, leading to the development of islands with complex internal compositional distributions (and hence complex internal strain states). A number of experimental studies have observed this strain-driven alloying in the Ge/Si [1] and InAs/GaAs [2,3] semiconductor systems. It is the aim of this work to develop a 2D simulation of the evolution of these islands during growth to gain insight into the processes by which these structures relax. This requires a novel multi-component model for surface and (near-surface) bulk diffusion under the influence of elastic strain. Such a model is outlined below with some initial benchtesting examples.

THE BASIC MODEL

The geometry is described within an hexagonal grid of cells (or lattice of atomic sites). We assign an occupancy probability, $p(i,j)$, to a cell (i,j) and allow it to evolve statistically as a continuous variable. The occupancy probability of each cell is then evolved at a rate given by the flux between the cell and its nearest neighbours. This flux is determined from a simple atomistic hopping model. Assume that each cell (lattice site) can either contain an atom or not. An atom is only allowed to move to an adjacent cell if that cell is unoccupied and has one or more other nearest neighbours, i.e. an atom cannot leave the surface. The activation energy for a jump is equal to $2Kn$ where K is the half-bond energy and n is the number of nearest neighbours (1 to 6). This is an initial state model, i.e. the activation energy does not depend on the final state. This approach is commonly adopted within kinetic Monte Carlo simulations and ensures that the rate and probability of a hopping event is completely determined by only the atoms six nearest neighbours. There are consequently 2^6=64 different atomic configurations local to a cell. The flux between each cell is calculated as the product of the transition rate and probability of a particular configuration summed over all possible configurations. The probability of each local configuration is determined from the occupancy probabilities of the six nearest neighbour cells. Despite the simplicity of these rules, complex behaviour representative of that seen in real physical systems can be produced. Figure 1 illustrates a simple test simulation for surface diffusion is a single-component system.

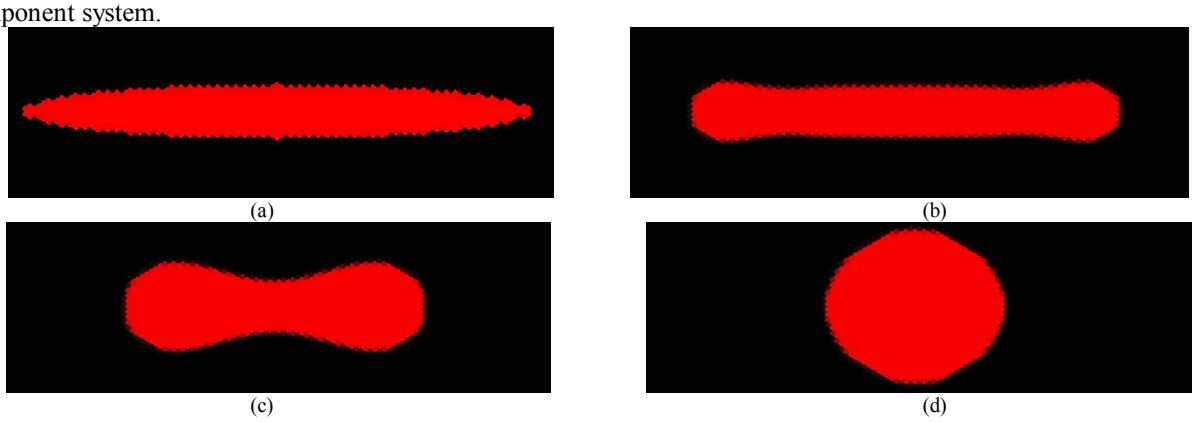

Figure 1. An ellipse evolves into a circle via surface diffusion to reduce its surface energy for K=1. (a) initial shape, (b) the high curvature ends quickly become more rounded, (c) the body gradually becomes more rounded over time, (d) the final stable state.

MULTI-COMPONENT SYSTEMS

The advantage of cellular automata is that they can readily be implement into a numerical simulation and it is easy to add additional physics. Here the previous model is easily extended to include two different components, A and B. There are now two state variables, $p_A(i,j)$ and $p_B(i,j)$, the probabilities that a cell (i,j) is occupied by an atom of A or an atom of B respectively. The transition rates subsequently depend on the different types of bond. $K_{AA,}$ K_{AB} and K_{BB} are taken to be the half-bond energies of the A-A, A-B and B-B bonds respectively. The average mass fluxes between each cell are determined from the sum of the probability weighted transition rates over all possible configurations as before. The introduction of more material parameters leads to a wealth of different phenomena. A simple illustration of one case of two-component diffusion is shown in Figure 2.

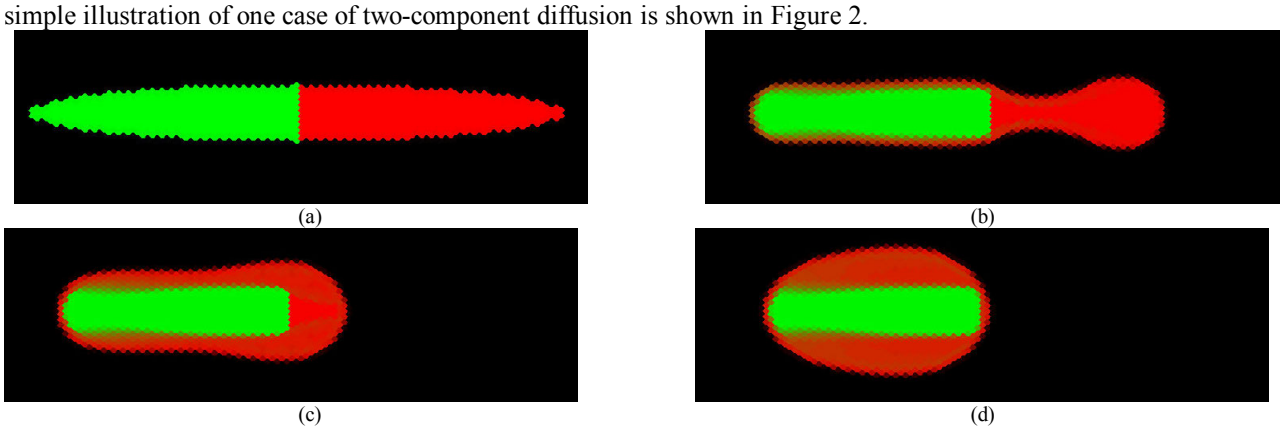

Figure 2. Evolution of a two-component elliptical body with K_{AA}=1.0, K_{AB}=1.2 and K_{BB}=1.4. Component A is red and B is green. (a) initial state, (b) A is more mobile than B, hence the low energy A surface quickly envelops B to remove the high energy B surface. (c) the evolution continues and (d) the body starts to become more circular.

ELASTICALLY STRAINED SYSTEMS

The bond energy is now a function of bond strain, ε. Assuming linear elasticity, the bond energy is modified to $K = K_0(1-\alpha\varepsilon^2)$. The forces between each cell due to the elastic term (weighted by the relevant cell occupancy probabilities) are equilibrated locally every iteration. They are equilibrated globally every 2000 iterations. The cell occupancy probabilities are evolved as before but with the strain dependent activation energy. Consequently, atoms in highly strained regions are more mobile than those in less strained regions. An example is shown in Figure 3.

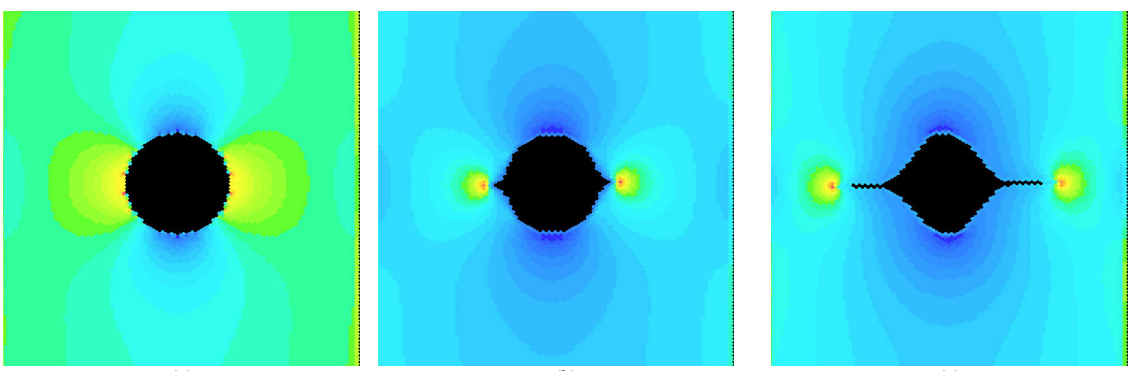

Figure 3.Evolution of a void in an elastically stressed body for K_0=1, α=6000 and an applied strain of 0.3%. (a) The plate is under uniaxial tension in the vertical direction. (b) Material flows over the surface of the void from areas of high elastic energy (red) to areas of low elastic energy (blue) causing small notches to appear on the side of the void, (c) the stress is raised at the notch tips causing them to grow into crack-like features.

CONCLUSION

The necessary mechanisms required to develop a model for coherent heteroepitaxial systems have been demonstrated. These features will be combined into one simulation to investigate the problems discussed in the Introduction.

ACKNOWLEDGEMENTS

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References

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