309b Developing a Reduced Order State Space Model for a Thin Film Deposition Process

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III-V semiconductors, such as gallium arsenide (GaAs), are used to manufacture a large variety of electronic and optoelectronic devices [1]. Molecular beam epitaxy (MBE) is a method that is widely used to grow GaAs thin films and nanostructures with high precision. However, because of the complex dynamics involved and the inherent control problem originating from the non-equilibrium growth, optimization of the characteristics of these structures is a challenging task.

Detailed Monte Carlo (MC) simulation models have been developed to describe the surface evolution during thin film deposition of GaAs by using scanning tunneling microscopy measurements [2] and density functional theory calculations [3]. We use the model of Itoh and his co-workers [2] in our kinetic Monte Carlo (KMC) simulations, since it describes the evolution of a wider range of surface configurations during growth.

In this study, a data driven approach is followed to obtain a state space model, which relates the input to the state of the system [4]. Firstly, the state space is explored by generating surface configurations under different inputs (e.g. gallium flux) and each configuration is characterized by using a special step-step correlation suitable for the zincblende lattice structure of GaAs. Then, the dimension of this KMC data is reduced by principal component analysis (PCA), and similar surface configurations are grouped using self-organizing map (SOM). Using these results, cell-to-cell mapping [5] is employed to characterize the transitions between different regions of the state space and a state space model is built by performing system identification.

The results of the system identification will be used in optimization and control of this thin film deposition process. Another goal in this study is automating the process of obtaining reduced order models from stochastic simulations.

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