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Process Engineering for Large-Scale Manufacturing of Compound Semiconductor Nanostructures

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This seminar will focus on the design and optimization of reactors that are used for (a) epitaxial growth of single crystalline thin films and (b) template-assisted growth of nanocrystals of compound semiconductors.

Thin films of compound semiconductors and multi-layer structures with atomically-abrupt interfaces form the basis of modern optoelectronic devices. The design of reactors for the epitaxial growth of single-crystalline films with uniform thickness and composition over large-area substrates, while maximizing the utilization of the expensive and toxic film precursors, is a very challenging problem. The process involves complex transport phenomena that are coupled with gas-phase and surface reactions on the surface of a substrate, where the film is deposited. We will discuss how fundamental process models can enable optimal design of vertical rotating-disc reactors used for metalorganic vapor phase epitaxy of III-V semiconductors, such as arsenides, nitrides and phosphides of Al, Ga and In. The initial focus will be on the development of generalized design criteria that guarantee recirculation-free flows, which are essential for growing multilayer structures with atomically-abrupt interfaces. We will subsequently discuss the development of detailed design maps that identify optimal operating conditions leading to uniform film thickness and composition. The models will be validated by comparing predictions from numerical simulations of laboratory- and industrial-scale reactors to experimental data.

Semiconductor nanocrystals of II-VI semiconductors, such as CdSe, ZnSe, ZnS and core/shell structures based on them, have unique optoelectronic properties that can be tuned by manipulating their size and composition. They are ideal materials for a variety of applications, including biological sensing and imaging, solar energy conversion, and ultra-high-color-definition displays. However, the large-scale manufacturing of these nanocrystals is very challenging, because typical laboratory-scale batch synthesis techniques are not amenable to scale up. We will discuss a new scalable technique for growing and doping II-VI nanocrystals using microemulsions and liquid crystals as templates. Stochastic simulations of the process have elucidated the underlying mechanisms of particle nucleation and growth and led to generalized scaling laws that govern particle coalescence in confined domains. Density Functional Theory calculations provided key insights on the thermodynamic stability of the nanocrystals and doping mechanisms. New reactor designs for continuous large-scale synthesis of nanocrystals will be discussed. Applications of ZnSe-based nanocrystals in the development of novel optical biosensors that are suitable for rapid point-of-care diagnostics will be discussed.