Kinetic simulation of Metastable Solvent Epitaxy

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Metastable solvent epitaxy (MSE) method is quite unique process, whose system configuration is similar with the traveling solvent method. The concentration gradient mainly controls the process. In this research, using the lattice gas model, the atomistic scale simulation of the epitaxial growth is performed. The kinetic of this process is governed by three different processes; detachment of solute atom from the interface of the feed, solute atom transport in solvent, and attachment of solute atom onto the interface of the seed. The solute atom transport in the solvent is mainly controlled by diffusion due to the suppressions of the convection flow in the thin liquid film.

The target of current research is the attachment or detachment mechanism of atoms, thus the diffusion rate is just adjusted by the vacancy density in lattice gas liquid. Considering that the atomistic level process is governed by the phase diagram, the attachment/detachment selection is just determined by the concentration of the liquid layer next to the interface of seed or feed. If the detaching solute dissolves into the higher concentration than the solubility limit, it goes back to the solid, and vice versa.

We are performing larger and longer scale simulations and will give the results at the conference.