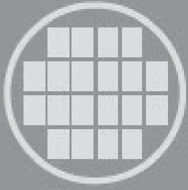
reaction DESIGN



CHEMKIN-PRO

Atomic Layer Deposition
Materials Processing for Electronics

Atomic Layer Deposition (ALD) is used to deposit thin films of solid materials in a controlled manner, exposing the deposition surface to pulses of alternating gases. Ideally, the deposition chemistry in ALD is self-limiting, with growth occurring in a layer-by-layer manner and the deposition thickness being controlled only by the number of cycles. The pulsed layering process of ALD leads to challenges that include ensuring adequate reaction to cover the substrate while controlling costs due to expensive precursor materials. CHEMKIN-PRO offers models for optimizing the pulse sequences of ALD and considering the effects of finite-rate kinetics for surface reactions, leading to saved time and money and a greater understanding of the processes involved.

Setting Up a Dynamic ALD Simulation

Pulsing of the chemicals into the system prevents many reactions in the two simulation systems set up here: one Perfectly Stirred Reactor, which runs quickly and serves as a quick check of the chemical reaction mechanism, and a Transient Stagnation Flow Reactor, which more realistically simulates a production-scale shower-head ALD reactor, including transport effects. This example demonstrates four cycles of the flow sequence including: metal-organic precursor in argon; argon purge; ozone in oxygen and argon; and argon purge. The chemistry set used here describes the atomic layer deposition (ALD) of alumina from trimethylaluminum (TMA) and ozone. This mechanism is deliberately simplistic, for illustration purposes only. It demonstrates one way of describing the ALD of alumina, but it should generally be considered as illustrative only and not used as a source of kinetic data for this process.

The chemistry set used here defines three surface species. There are only three surface reactions:

- The dissociative adsorption of TMA on the oxygenated surface species O(S) to form ALME2(S), combined with the recombination of two methyl groups and desorption of an ethane molecule.
- Gas-phase oxygen atoms reacting with the two ALME2(S) to form the ALMEOALME(S) species and a gas-phase ethane molecule.
- An O atom reacting with the ALMEOALME(S) species to deposit AL2O3(B), regenerate O(S), and form gas-phase ethane.

Results

By the end of the TMA pulse, all the TMA flowing into the reactor is also flowing out again.

For the oxidizer pulse, the contour plot of O atom mole fractions in Figure 1 show how the O atoms are formed by gas-phase decomposition of ozone in the hotter regions of the gas, and then react away, at the surface. The site fractions in Figure 2 show that the methylated surface species (ALME2(S) and ALMEOALME(S)) are not completely converted to O(S) during the oxidizer pulse. This probably results from the fact that the oxidation occurs as two sequential steps and the kinetics are limiting the process. The plot of O atom mole fractions in Figure 3 shows that the O atoms are not being depleted at the surface in the stagnation flow simulations, which suggests a kinetic limitation, possibly resulting from the default reaction orders in this simple mechanism. The incomplete oxidation of the methylated surface species in turn leads to less than unity O(S) coverage at the beginning of the TMA pulse, which in turn leads to less efficient use of TMA and some notable differences between the first and subsequent pulses.

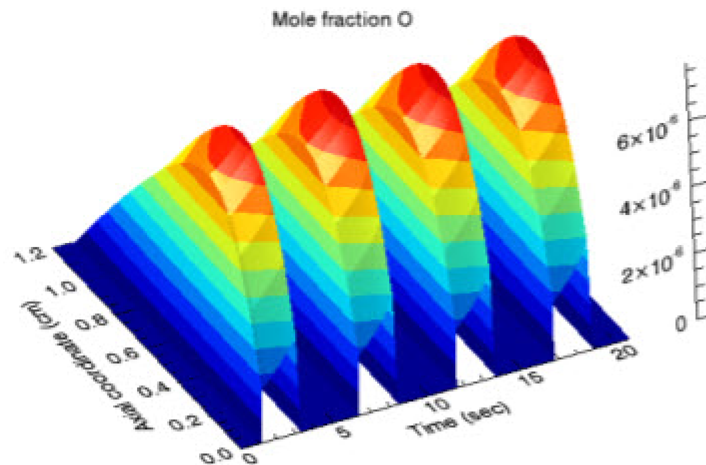


Figure 1. O mole fraction: O atoms from ozone form in hot regions and react at surface.

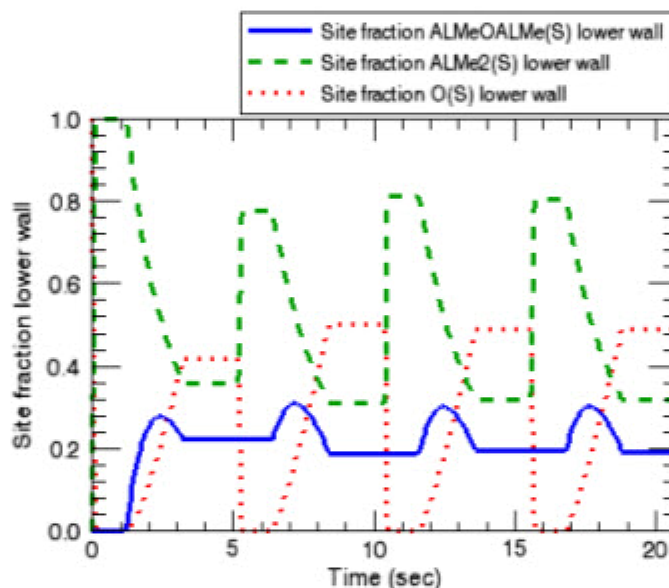


Figure 2. Stagnation-flow site fractions: methylated surface species incompletely converted.

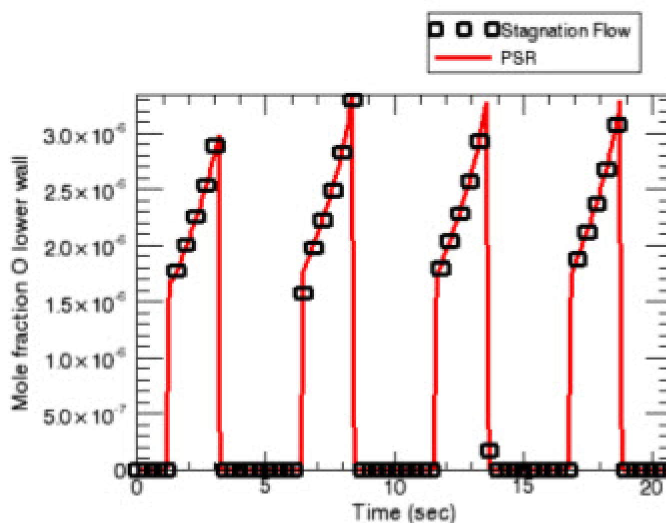


Figure 3. O mole fractions comparison: O atoms undepleted.

©2013 Reaction Design. Reaction Design and CHEMKIN are registered trademarks of Reaction Design.
FORTÉ, ENERGICO, CHEMKIN-PRO and CHEMKIN-PRO Reaction Workbench are trademarks
of Reaction Design. All other trademarks are the property of their respective owners.