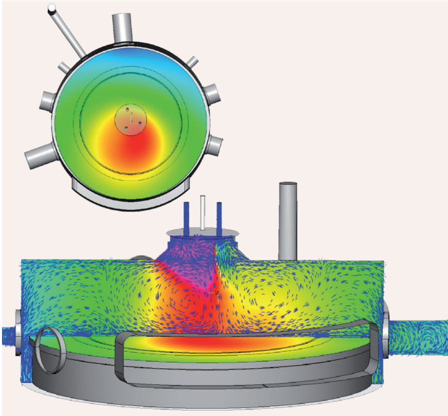
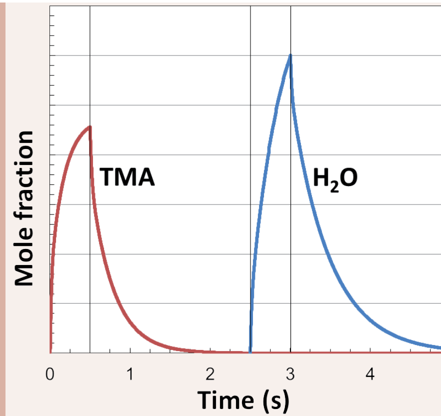
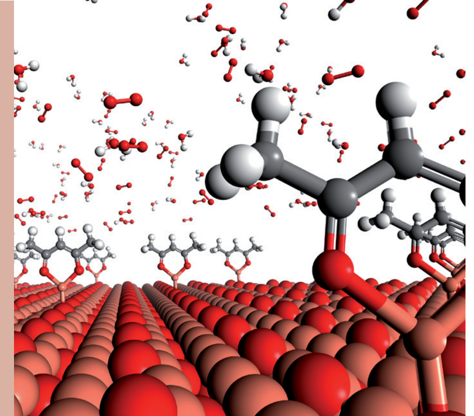
MULTI SCALE SIMULATION OF ATOMIC LAYER DEPOSITION







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Figures: H_2O distribution for Al_2O_3 ALD in reactor (left) and on wafer surface (left inset); TMA and water concentration during ALD cycle (center); Atomic scale ALD simulation (sketch, right)

Photo acknowledgments: Fraunhofer ENAS
All information contained in this datasheet is preliminary and subject to change. Furthermore, the described systems, materials and processes are not commercial products.

Reactor scale simulation including ALD chemistry

Fluid dynamics in ALD reactors

- Coupled calculation of
  - Gas flow
  - Distribution of species
  - Temperature
  - ALD reactions (surface and gas phase chemistry)
- Prediction of
  - Growth per cycle
  - Optimal dose/purge times
  - Layer composition and homogeneity
  - Optimal reactor design
- Time-dependent simulations
- Arbitrary reactor geometry
- 2D and 3D models
- Methods
  - CFD (computational fluid dynamics)
  - MC (Monte Carlo approaches)

Examples

- Al_2O_3 from TMA and H_2O
- TaN from PDMAT

Atomic scale modeling and film growth simulation

Properties of precursor molecules

- Screening of different precursors
  - Thermodynamic properties
  - Thermal stability
  - Preselection of promising precursors

Surface and gas phase reaction simulation

- Reaction kinetics
  - Reaction pathways
  - Reaction rates
- Input for reactor scale simulation → multiscale approach
- Methods and software
  - DFT (density functional theory)
  - RMD (reactive molecular dynamics)

Examples

- Dissociation of Cu(I) precursor on Ta
- Dissociation of Cu(II) precursor on various substrates
- Stability and reactivity of Cu precursors in gas phase

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