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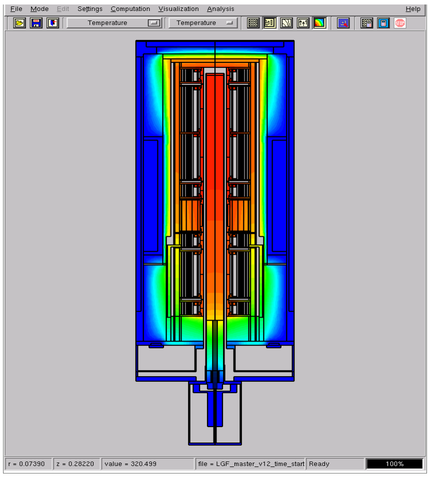
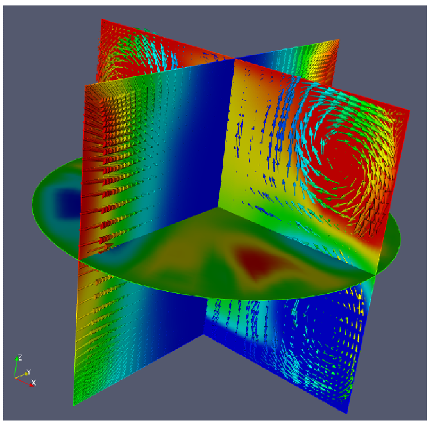
FRAUNHOFER INSTITUTE FOR INTEGRATED SYSTEMS AND DEVICE TECHNOLOGY IISB

Equipment Simulation for Crystal Growth and Semiconductor Technology



Global simulation with CrysMAS: computed temperature field in ESA's low gradient furnace operated onboard the International Space Station.



Local 3D simulation of melt flow with Openfoam: convective heat transport in a silicon melt due to electromagnetic stirring.

Equipment Simulation of Crystal Growth Processes

Fraunhofer IISB is using in-house developed software packages as well as commercial CFD software for optimizing equipment and processes for bulk crystal growth and alloy solidification, and for predicting crystal defects and microstructure formation.

For many years now, the software package CrysMAS of Fraunhofer IISB is well established in industry and academia in all fields of crystal growth, such as bulk growth of semiconductor, fluoride, and oxide crystals by Czochralski, Bridgman, and gradient freezing methods. CrysMAS is tailored to solve global heat and mass transport phenomena in high-temperature equipment with complex axis-symmetric geometry. It is well documented and provides an easy-to-learn, easy-to-use graphical user interface. Powerful numerical methods for solving inverse problems efficiently assist the user when optimizing equipment and processes. Comprehensive service is offered to the CrysMAS users, including tailored training on our software modules, user support, on-line documentation, and consultancy for your specific tasks. Due to our close link to experimental problems, we are able to continuously improve our software tools according to your needs.

CrysMAS offers a variety of physical models:
- Heat transport by (anisotropic) conduction, by laminar or turbulent convection (gas and melt), and by radiation between grey emitting surfaces and in absorbing media
- Magnetohydrodynamic phenomena (steady and time-dependent)
- Diffusive and convective mass transport
- Phase transitions
- Resistance and inductive heating

Furthermore, special models are implemented for:
- Moving furnace parts
- Thermo-elastic stress and dislocations in crystals
- Chemical reactions

For 3D simulations, either commercial CFD software or the open source package Openfoam is used at Fraunhofer IISB. The latter has proven to be well suited, especially for local simulations of the melt flow occurring during growth of silicon by the Czochralski technique and ingot casting. The availability of a high performance Linux cluster at Fraunhofer IISB allows massive parallel simulations, which are a prerequisite for accurately solving convective phenomena in 3D in reasonable times.

Equipment Simulation for Semiconductor Technology

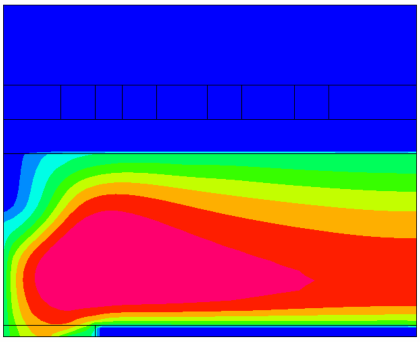
Semiconductor equipment simulation helps in developing and optimizing processes and equipment. The usage of commercial equipment simulation tools allows us to study a variety of equipment types, as used in semiconductor technology, among others:

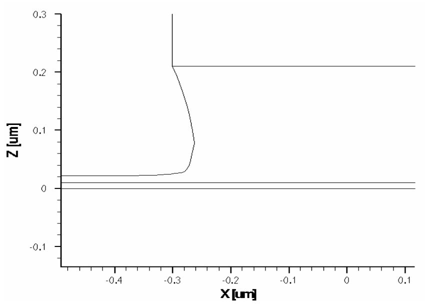
- Reactors for sputter deposition processes (conventional and long-throw), with and without ionized metal plasma
- Reactors for chemical vapor deposition, with and without plasma enhancement
- Equipment for thermal processes, such as rapid thermal processing (RTP) or oxidation
- Reactors for physical sputter etching and reactive ion etching (RIE)
- Other equipment types according to our customers' needs

Application examples include:

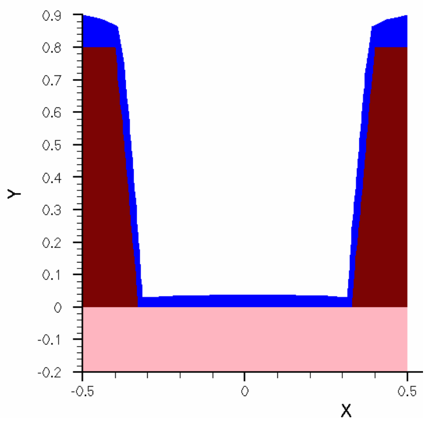
- Investigation of etch or deposition rates depending on the process parameters, such as pressure and gas flow, or electrical parameters of a plasma reactor
- Determination of non-uniformities across the wafer
- Investigation of gas flow through semiconductor equipment
- Investigation of the influence of geometrical modifications

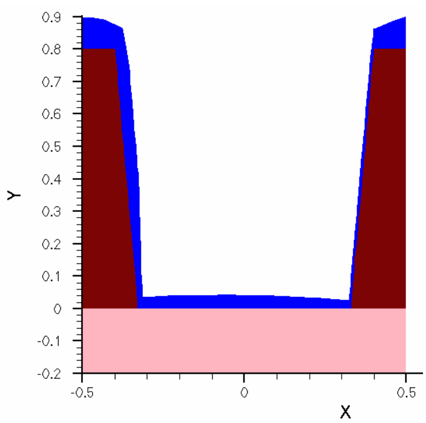
Furthermore, we use in-house and third-party feature-scale simulation tools that can read output from equipment simulation, such as species concentrations or angular and energy distributions of ions, and predict the resulting geometries on feature-scale, such as the conformality of a deposited layer or the profile of an etched trench. Also profile non-uniformities across the wafers can be studied. Our feature simulation tools treat fluxes of ions and neutrals, and determine the interaction with the substrate to predict local rates according to the mechanism of a particular process. Different mechanisms exist, ranging from purely physical or purely chemical etching to complexer ones, such as ion-enhanced desorption of etch products, re-emission of etching products or precursors, or passivating agents depositing on the feature surface.

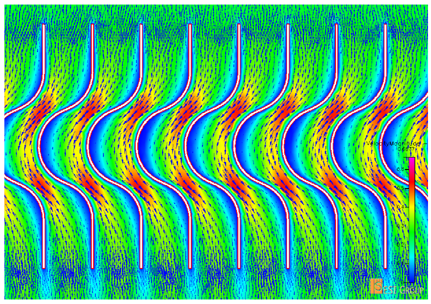




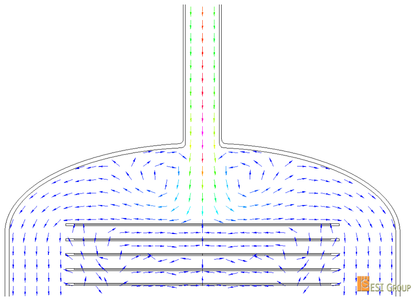
Simulated concentration of Cl_2^+ ions in a rotationally symmetric (rotation axis is on the left side) inductively coupled plasma etch reactor used for polysilicon etching (top). Simulated etched polysilicon feature profile at the center position of the reactor (bottom).







Simulated flow (vertical 2D cut) of clean room air through the top cover of a semiconductor manufacturing tool, in which a laser is in operation. The cover is designed to prevent direct light transmission.



Simulated inflow of nitrogen into a low-pressure plasma batch nitridation reactor (rotationally symmetric, velocity color coded from 0-50 m/s).

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Simulated profiles of Ti in a via resulting from long-throw sputter deposition. Via position: center of the wafer (top), rim of the wafer (bottom).