CGSim Crystal Growth Simulator

Software for Optimization and Process Development of Crystal Growth from the Melt and Solution

STR Group
About STR Group

Semiconductor Technology Research Group (STR Group) provides specialized software and consulting services for modeling of crystal growth, epitaxial process, and operation of semiconductor devices. Every consulting activity and software product is preceded by comprehensive research and careful validation of physical models and approaches applied.

Four product lines are developed by STR:

Crystal growth from the melt and solution
Modeling of crystal growth from the melt (Si, Ge, III/V, oxides, fluorides, halides) or solution (SiC) using different methods: Czochralski (and its modifications), DS, Kyropoulos, HEM, Bridgman, FZ, Flux Method and others.

Bulk crystal growth from the gas phase
Modeling of PVT, HVPE and HT-CVD growth of wide bandgap semiconductors (SiC, AlN, GaN, AlGaN). Available computer models include heat and mass transport in the reactor, crystal shape evolution, stress and defects dynamics, faceting.

Optoelectronic devices
Modeling of advanced semiconductor devices includes operation of LEDs, laser diodes, and solar cell heterostructures. Available models enable prediction of device characteristics followed by optimization of heterostructure and chip design.

Epitaxy
Reactor modeling: flow dynamics and heat transfer, diffusion, advanced chemical models deposition, parasitic reactions and gas-phase nucleation.
Process modeling: composition profile, strain distribution and dislocation density, surface chemistry, particle formation.
Overview of the CGSim package

CGSim (Crystal Growth Simulator) is a specialized software for modeling of crystal growth from the melt (Si, Ge, III/V, oxides, fluorides, halides) or solution (SiC) using different methods: Czochralski (and its modifications), DS, Kyropoulos, HEM (and its modifications), Bridgman, FZ, Flux Method and others. CGSim is used by more than 70 crystal growth companies all over the world, including giant manufacturers and much smaller research facilities and foundries. Simulations are mostly applied for process optimization in terms of crystal quality, energy consumption, and higher yields. In particular, the modeling can help in design and optimization of hot zones in order to grow larger and better crystals.

The tool is designed with process engineers and growers in mind and does not require a background in numerical simulations. It provides insight into some physical processes that are extremely difficult to monitor experimentally while their understanding can be crucial for optimization of the costs and further improvement of the crystal yield and quality.

CGSim package includes several modules: CGSim-2D, Flow Module-3D and Cz Dynamics:

- **CGSim-2D**: Global heat transfer, laminar and turbulent flows, DC and AC magnetic fields, advanced radiative heat transfer, species transport, dynamics of the melt/crystal interface, thermal stresses, point defects dynamics, formation of voids and oxygen precipitates, advanced control of crystal growth process. Smart visualization tools.

- **Flow Module-3D**: Unsteady 3D modeling of heat transfer and convection during melting and crystal growth:
  - Crystallization front geometry;
  - Probability of crystal twisting;
  - Probability of single structure loss related to local temperature fluctuations under the crystal;
  - Transport of oxygen and other impurities in the melt and gas

- **Cz Dynamics**: Transient modeling of Cz Si growth coupled with point defect dynamics:
  - Crystallization front evolution during the crown and tail growth;
  - Segregation of impurities and dopants;
  - Dynamics of point defects in transient thermal field;
  - Multiplication of dislocations
What practical problems can be solved with CGSim?

- Reduce electricity consumption
- Increase crystal growth rate keeping crystal quality
- Reduce probability of monocrystalline structure loss
- Achieve the required concentration of impurities and dopants
- Control thermal stresses and defects in growing crystals
- Reduce impurity deposition on furnace elements
- Increase the lifetime of furnace elements
- Increase grain size in multicrystalline silicon ingots
- Avoid ‘dark clouds’ in silicon ingots
- Reduce bubble concentration in sapphire crystals
- Reduce dislocation density in crystals
- Optimize seeding stage to reduce the time of seeding
- Optimize crystal cooling stage
CGSim-2D: foundation of the package

CGSim-2D package is developed for industrial and academic research teams. Graphical User Interface of CGSim does not require special computational skills. Problem definition and parameter specification are highly automated to minimize user’s efforts and time. High flexibility in definition of geometry and boundary conditions make CGSim a versatile tool for modeling of different growth processes (see the interface screenshots on page 4).

Geometry import from AutoCAD is supported. Auto grid generator with support of mismatched block interfaces enables quick generation of computational grid in the entire computational domain. The software automatically reconstructs the geometries of crystal, melt, and encapsulant in Cz and LEC growth processes for various crystal positions enabling serial computations. Calculation of meniscus surface for the melt and encapsulant is available. Material properties are stored in a special database.

The solver of Basic CGSim enables computation of coupled problem of heat transfer, laminar and turbulent flows, electromagnetic effects, thermal stresses and transport of species. Ready chemical models for impurity transport in Si growth processes are included into the software package.

Both quasi-steady and transient computations can be performed. Process control procedure enables automatic adjustment of heater power to achieve the target growth rate or temperature in multiple control points for multi-heater configurations.
 Convenient visualization tools allow analysis of 2D distributions of different variables. Boundary tool enables easy extraction of 1D plots of variables along the boundaries including distributions of heat and mass fluxes, V/G ratio and temperature gradients along the crystallization front. Point, line and time probes are available. Animation tools help to understand features of transient processes. Special tools enable extraction of high quality images and animations.

**Cz Dynamics** module is designed for transient modeling of Cz crystal pulling process. Heater power profile can be automatically adjusted to follow target crystal pulling rate. The user can specify time dependent crystal and crucible rotation rates as well. Computation is coupled to modeling of self-defects dynamics in the growing crystal.

**Flow Module-3D**

Flow Module-3D is designed for professional 3D analysis of turbulent and laminar convection in the crystallization zone. A unique approach is used to couple this analysis with the global heat transfer. Tools for the automatic generation of 3D grids without singular cells on the basis of a 2D grid and control of grid quality are included. The user can choose the RANS, LES/URANS, DNS, or quasi DNS approaches and apply a model of turbulence specifically adapted for the melt turbulent flow computations. Radiative heat transfer in semitransparent blocks can be accurately considered. Advanced approximations of convective and diffusive terms allow the application of coarser computational grids and perform faster analysis.
Global Heat Transfer

Engineering model of global heat transfer in Cz systems that is currently used in CGSim includes self-consistent calculation of melt turbulent convection, inert gas flow and melt-crystal interface geometry. The model of global heat transfer is presented in [V. V. Kalaev, et al, J. Crystal Growth, 249/1-2 (2003) pp. 87-99]. The predicted temperature distribution (bottom left) is compared to the experimental data (right) obtained in the points shown in the reactor scheme (bottom right).
Species transport

Ready-to-use model of impurity transport in Cz Si growth is available in CGSim software. The model includes all important reactions required for accurate modeling of species transport in the melt: oxygen and carbon and in gas: CO, SiO and silicon vapor. Impurities in gas are actively interacting with furnace elements with formation of deposition layers. CGSim includes a proprietary model defining one of three different types of deposition depending on the surface temperature and gas composition.

Defect analysis

Accurate analysis of temperature gradients (a) and thermal stresses (b) is possible in CGSim and in Flow Module. For Cz Si growth, there are 2D/1D calculations of intrinsic defect incorporation, recombination, and clusterization. The difference between vacancy and interstitial concentrations (c) shows the type of dominating defects and the position of OSF ring.
Cz Dynamics

Cz Dynamics is a component of CGSim package designed for transient modeling of crystal pulling process. The tool incorporates automatic algorithm of heater power adjustment to follow user-defined crystal pulling rate profile. Within Cz Dynamics, it is possible to analyze such complex phenomena as transition from crown to cylinder, and effect of variable crystal pulling rate on distribution of vacancies and interstitials and on location of OSF ring in the crystal.

Cooling stage optimization

Optimization of crystal cooling stage helps to considerably reduce the process cycle and increase productivity of crystal growth furnace. In CGSim software it is possible to develop optimal moving profiles for the crystal and crucible (with constant or variable moving rate), and heater power recipe for the cooling stage. The target is to reduce the cooling time keeping a low level of thermal stresses in the crystal and keeping the melt from abrupt solidification.
**3D Modeling**

To predict the geometry of the melt-crystal interface quantitatively, we use 3D unsteady analysis of melt turbulent convection coupled with the heat transfer analysis in the crystal and the crucible. 3D grid is built for the crystallization zone including the melt, crucibles, and the crystal (left). Flow Module-3D of CGSim has been used to predict the geometry of the crystallization front for 100 mm crystal (right) and for 300 mm crystal [D.P. Luknin et al, J. Crystal Growth, 266/1-3 (2004) pp. 20-27.

![Graphs showing interface deflection vs radial position for 100mm and 300mm crystals](image)

**DC Magnetic Fields in 400 mm Cz Si**

Increase in the crystal diameter necessitates the control over the turbulent natural convection in large volumes, which is often achieved via magnetic fields (MF). Application of MFs changes heat transfer and convection patterns in the melt.

![Graphs showing temperature distribution with and without MF](image)

Presented example shows that application of cusp MF of 30 mT suppresses turbulent fluctuations and melt flow at the melt periphery, while mixing of the melt under the crystallization front remains strong. Presented example shows that application of cusp MF of 30 mT suppresses turbulent fluctuations and melt flow at the melt periphery, while mixing of the melt under the crystallization front remains strong.
Strong horizontal MFs nearly completely suppresses melt flow in a cross-section positioned along the induction vector, leaving high velocity flows in the cross-section positioned orthogonal to the magnetic induction vector. One can also notice substantially asymmetric temperature distribution at the melt surface and an upward flow of the melt in the area located under the crystal. This upward motion results from combined effect of MFs and Ar flow.

**Directional Solidification (DS) of Si for PV**

**Global Heat Transfer** CGSim software performs unsteady modeling of silicon crystallization in directional solidification and VGF furnaces from heating up to ingot cooling stage, taking into account moving insulations (bottom left) [B. Wu et al, J. Crystal Growth, 310/7-9 (2008) pp. 2178-2184], and variations of heater power to obtain target temperature recipe in control point, or target crystallization rate. Computations are coupled with moving melt/crystal interface shape (bottom right) both for traditional multicrystalline process, and for process with partial melting of the feed stock and/or seed crystals.
Illustration at the bottom of previous page presents a very good correlation between experimental and calculated crystallization interface shapes.

**Dislocations and residual stresses.**
Alexander-Haasen model is implemented in CGSim package for unsteady analysis of crystal plastic deformation due to thermal stresses with generation of dislocations. The model can also be used for optimization of crystal cooling stage to find optimal balance between the cooling time and dislocation density/residual stresses. The model provides a good agreement with published experimental measurements of residual stresses in mono-like silicon both for mono and multi-crystalline parts (right top) [O. Smirnova et al/Cryst. Growth Des. 2014, 14, 5532–5536].

**Transport of species**
CGSim package includes built-in model of species transport taking into account chemical reactions at different surfaces and in the volume (right center). Chemical model includes transport and incorporation of oxygen, nitrogen and carbon into the crystal, and three different types of deposition at the furnace walls. The model also calculates formation of SiC, Si₃N₄, and Si₂N₂O particles in the melt.

2D (right center) or fully 3D (right bottom) unsteady approximations can be used for modeling of species transport.
The model of carbon segregation (top) was successfully verified and used for technology optimization in [Y.Y. Teng et al, J. Crystal Growth, 312/8 (2010) pp. 1282-1290]. The authors report 10% decrease of carbon concentration in the crystal by using CGSim modeling results, which was obtained by modifying the melt flow pattern and crystallization interface shape.

**Kyropoulos sapphire crystal growth**

Sapphire crystal growth systems are characterized by high temperature values and a great challenge in obtaining experimental data about the process. In this situation, numerical modeling is a very efficient approach for analysis and optimization of crystal growth technology.

Computational approaches available in CGSim software take into account turbulent flow of the sapphire melt, laminar gas flow, and radiative heat exchange in the semi-transparent crystal including specular reflectivity at the boundaries, internal absorption and scattering.

**Heat transfer in the furnace** Global heat transfer in a Ky furnace is strongly affected by number, location and sizes of molybdenum heat shields (right). The aim of heat shield optimization is to develop a hot zone with optimal temperature distribution around the crucible and growing crystal to enable crystal growth with stable diameter and low thermal stresses.

**Model verification** The model was verified using available experimental data. CGSim software could successfully reproduce spoke-like temperature pattern induced by Marangoni forces observed in experiment at the melt free surface (next page, top left).
A good agreement between the crystallization shapes predicted via computations and those observed experimentally indicates that the model provides an adequate prediction of the temperature and heat fluxes in the crystal and in the melt. This ensures numerical prediction of the thermal stresses generating dislocations in the crystal (top right).

**Example of industrial application: furnace optimization**

Optimization of Kyropoulos furnace design helps to decrease temperature gradients in the crystal and improve crystal quality and yield. Using the CGSim package, several configurations of the industrial furnace have been considered. In the initial configuration (left) melt flow pattern provided direct delivery of the hot melt to the crystallization front, resulting in high temperature gradients along the melt/crystal interface. After considering several hot zone modifications, we found a furnace configuration providing one-vortex flow structure in the melt (right). Such flow pattern results in gradual cool-down of the melt and up to 30% decrease of the temperature gradients in the crystal. Temperature gradients inside the crystal and thermal stress values have been significantly reduced (below).
Improvement of the crystal quality has been confirmed experimentally. Morphological and optical investigation of wafer samples obtained in the upper part of the crystal has shown that the dislocation density in morphological R-plane after modifications dropped from $10^3 \text{ cm}^{-2}$ to $10^2 \text{ cm}^{-2}$, (below).

**Example: 3D modeling of Ky sapphire growth in 250 mm diameter crucible.**

Crystal seeding is successful only if there is a stable local temperature minimum in the point of seeding at the melt free surface. 3D unsteady modeling of the melt convection and crystallization helps to find optimal heating conditions for stable seeding and shoudering stages. Examples of the melt flow instability at the free surface at initial stages are presented at the right [S.E. Demina et al, J. Crystal Growth 320 (2011) pp. 23–27 13, 14].
HEM Sapphire crystal growth

HEM sapphire growth technology is characterized by a high level of process automatization. In these conditions, a well developed hotzone design and process recipe become the key factors to grow high quality sapphire boules. Unique approaches developed in STR enable fully unsteady computations of HEM sapphire crystal growth process with precise modeling of radiative heat transfer in the crystal and careful account of the gap between the crystal and the crucible (a).

Bubbles Incorporation of bubbles into the crystal is closely related to the melt flow structure and intensity. CGSim software accurately calculates the melt flow, taking into account the effects of natural convection and Marangoni forces (b).

Dislocations and residual stresses CGSim software provides modeling capabilities to calculate thermal stresses and their release into dislocations within Alexander-Haasen model due to plastic crystal deformation. Generation of dislocations and residual stresses (bottom) can be calculated both during crystal growth and cooling stages in a single computation.
**SiC crystal growth from solution**

Top-Seeded Solution Growth (TSSG) of silicon carbide (SiC) is characterized by relatively low growth rate. Long and time-consuming experiments, make computer modeling an attractive option for optimization of crystal growth process.

**Global Heat Transfer and Flows** SiC crystal growth conditions are affected by heating of the crucible. Computer model includes calculation of heat transfer in entire crystal growth furnace, inductive heating of the crucible, automatic adjustment of electric current in inductor, and constant or accelerated rotation of crucible and seed. Modeling capabilities allow user to analyze different furnace designs and rotation parameters both in 2D and 3D to achieve efficient transport of carbon to growing crystal.

**Chemical Model of Carbon Transport**

with different solvents for silicon melt is built into the CGSim software, and can be used for calculation of crystallization rate value and its uniformity over the melt/crystal interface.

**VGF/Brigdeman growth of GaAs**

CGSim software can accurately calculate heat transfer in Bridgeman/VGF crystal growth furnace taking into account anisotropic furnace elements, melt, gas and encapsulant flows. Dynamics of the crystallization interface is coupled with global heat transfer and release of the latent heat.

**Heater powers** in unsteady computations can be automatically adjusted to achieve the required time evolutions of temperatures in control points, or crystal growth rate.
**Dopants** Modeling of melt flow is coupled with convective and diffusive transport of dopants. Incorporation of dopants into the crystal is calculated taking into account segregation effect. Two picture present examples of calculated dopant distribution in the crystal.

**Dislocation Density** Unsteady computation of VGF process in CGSim software is coupled to modeling of thermal stresses evolution in the crystal, and their relaxation with generation of dislocations. Since generation of dislocations happens both during crystal growth and cooling stages, such modeling analysis is also performed continuously during growth and cooling stages within a single computation.

Calculated results present distribution of dislocation density (left bottom) and residual stresses in the grown crystal. Computer model has been successfully verified against published experimental data (right bottom).
References
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