Semiconductor Technology Research Inc.

Use of *CGSim* package for analysis and optimization of Cz, LEC, and VCz growth of semiconductor crystals

P.O. Box 70604, Richmond, VA 23255-0604, USA
Tel: +1 804 304 8092 Fax: +1 804 754 2114
http://www.semitech.us
E-mail: cgsim@semitech.us

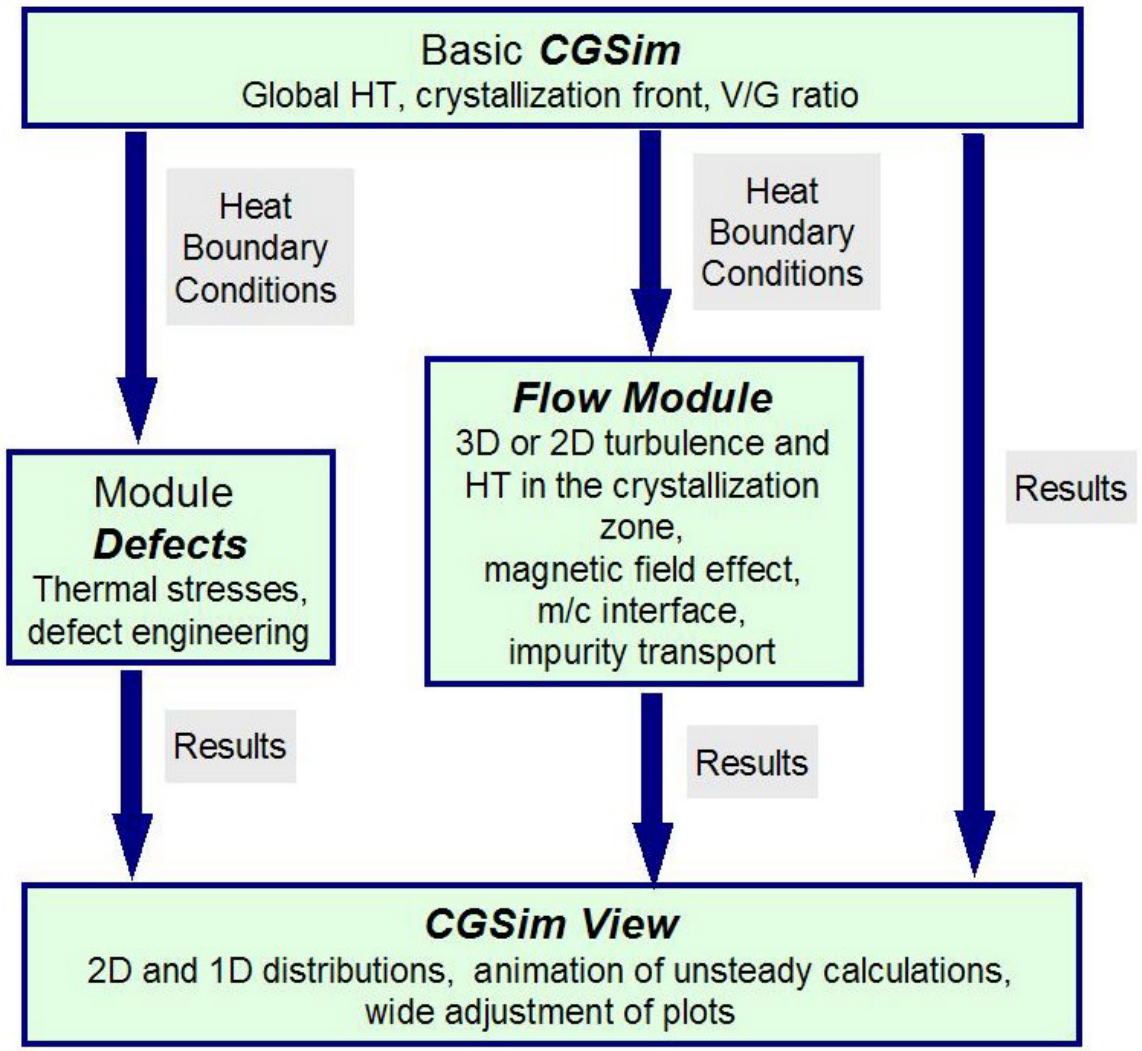
Problems to be resolved using *CGSim* software

1. Control of optimal geometry of the crystallization front by geometrical/material modifications of the hot zone of a growth system
2. Control of stresses and defects in growing crystal. Defect engineering with accurate adjustment of the heat shields
3. Governing melt convection by crystal/crucible rotation rates, magnetic fields of different strength and orientation. Stabilization of melt convection with keeping reasonable turbulent mixing
4. Analysis of impurity transport in the melt and in the gas. Prediction of oxygen and carbon containing species in Si CZ growth. Adjustment of growth conditions, modifications of hot zone to get desired impurity concentrations
5. Adequate account of encapsulant and turbulent gas flow in liquid encapsulated growth
6. Modeling support of the development of a new growth setup

***CGSim*:**

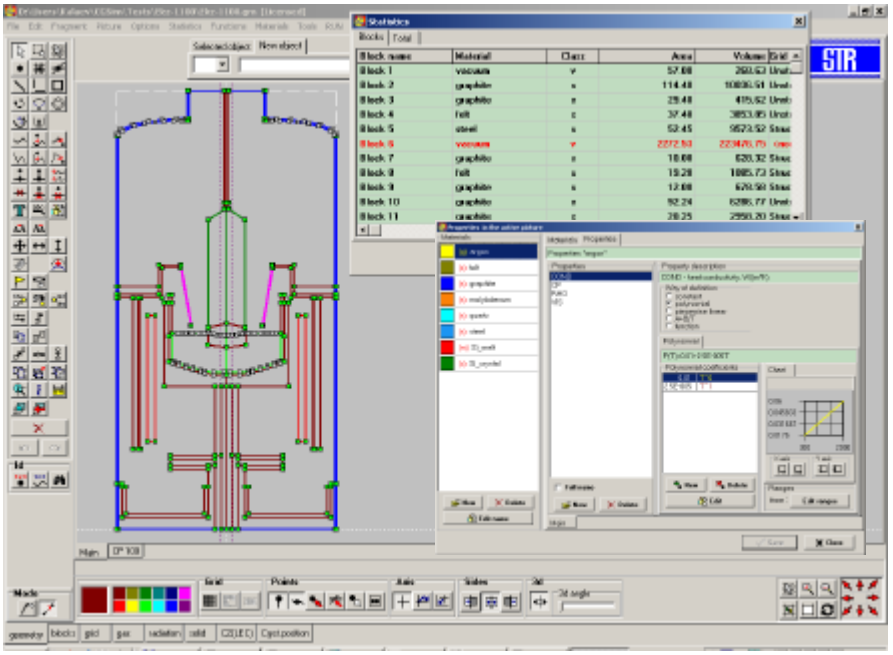
Fast and cheap development of industrial growth technology

Content of the ***CGSim*** package:

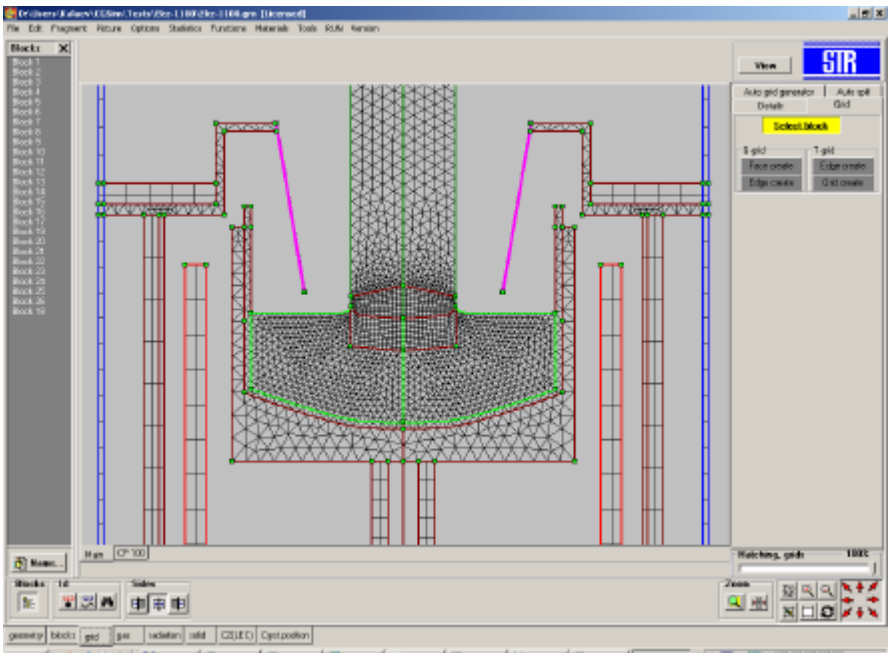


Basic *CGSim*

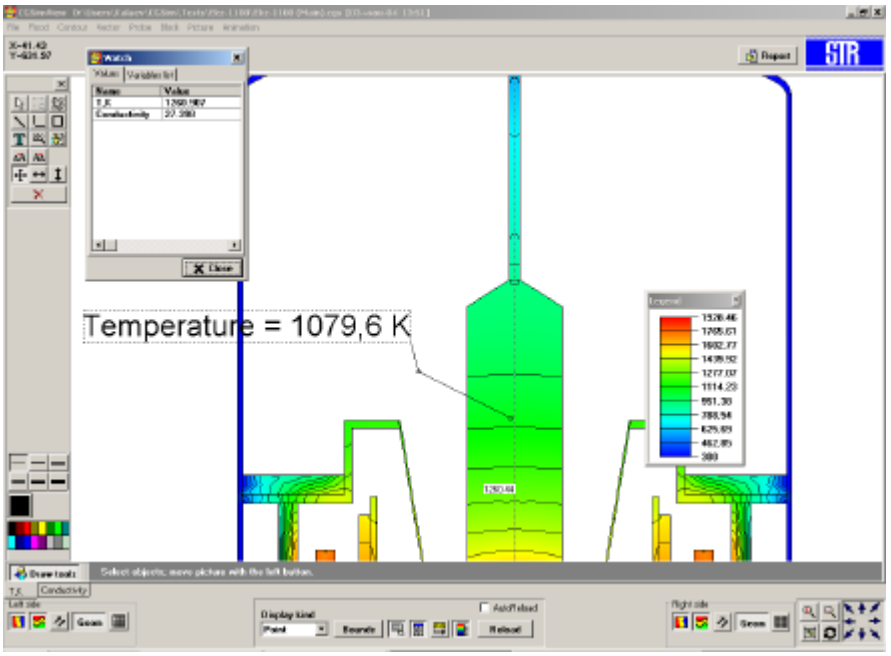
Basic module of Crystal Growth Simulator is specially desired for using in industry and research teams. GUI of ***CGSim*** is developed implying no special computational skills of users. All steps of a calculation are maximally automatized to decrease man power.



There is export from AutoCAD DXF files together with automatic tools for grid creation. Mismatched block interfaces for both triangular and rectangular grids are supported. Material properties are stored in a special data base. The calculation of meniscus of the melt and encapsulant surface are available as preprocessing. Thermal stress and defect distribution are predicted.

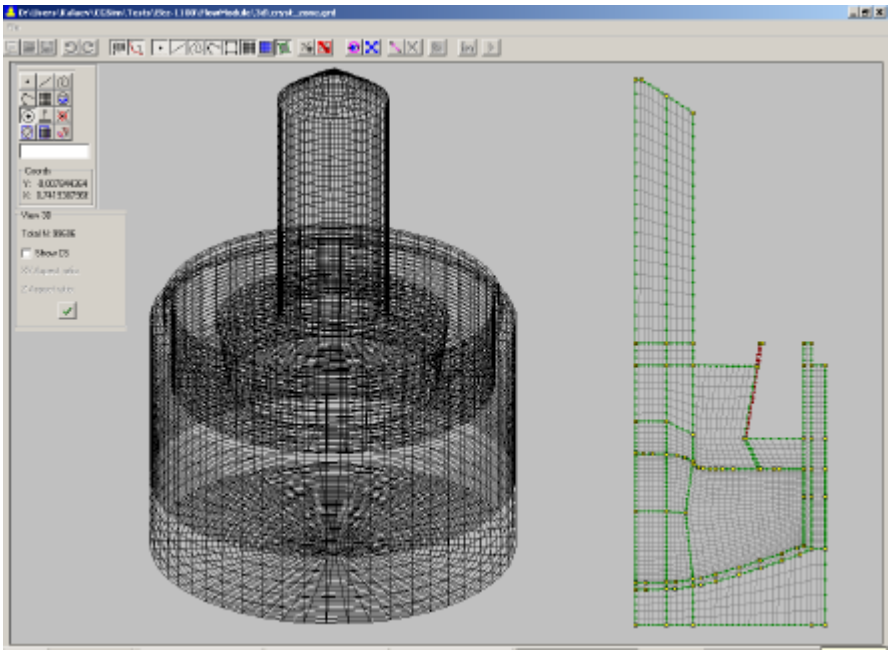


CGSim visualizer allows analysis of 2D and 1D distributions including heat & mass fluxes, V/G ratio and temperature gradient along the crystallization front. There are dynamic monitoring points, probe lines, surface distributions. Animation tools help to understand features of 3D melt convection. Special options are provided for the preparation of good quality pictures.

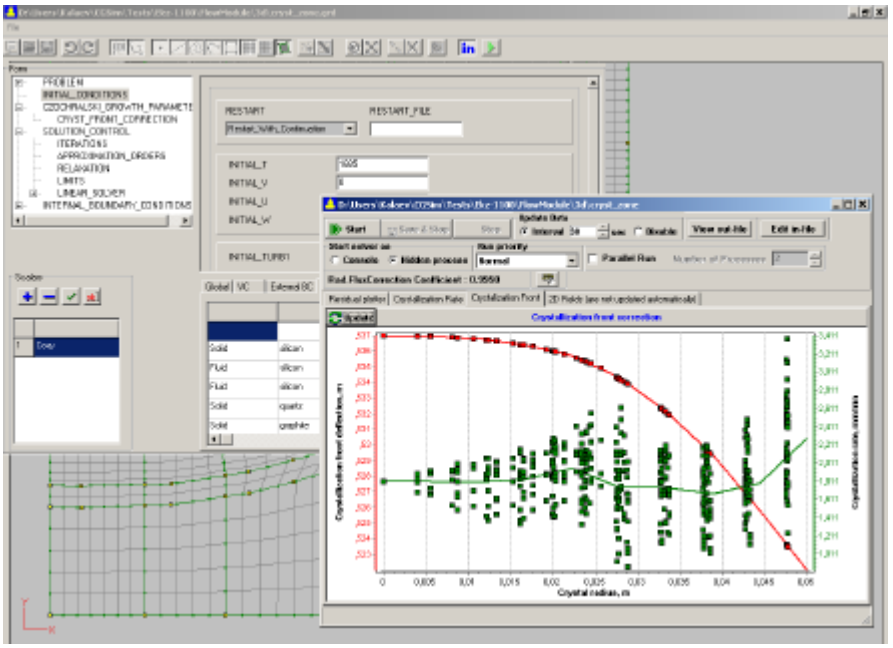


Flow Module

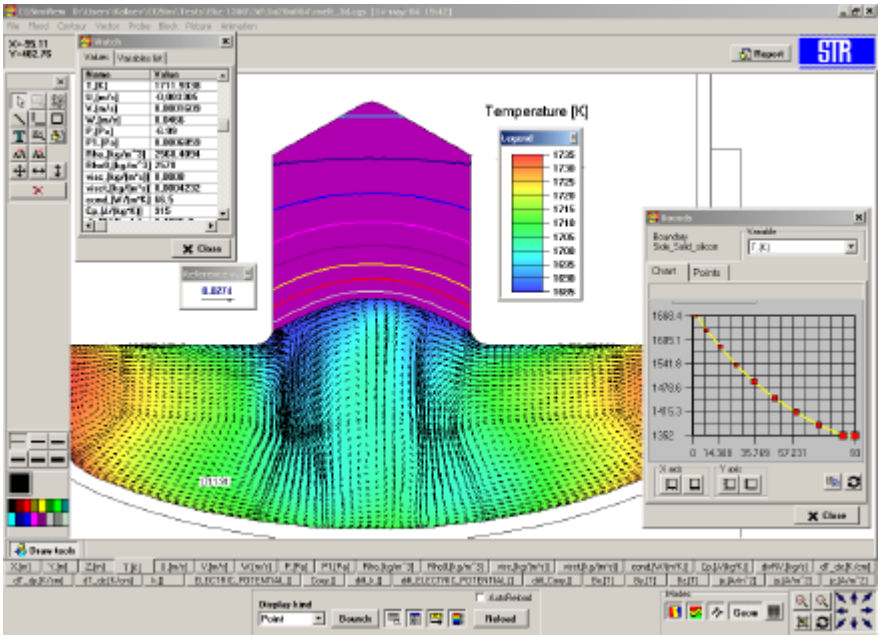
Flow Module is desired for professional analysis of 3D or 2D turbulent and laminar convection in the crystallization zone including the melt, crystal, crucibles, and gas or encapsulant domains. A unique approach is used to couple this analysis with global heat transfer. There are automatic generation of a 3D grid without singular cells on the basis of a 2D grid and tools for control of grid quality.



The user can choose the RANS, LES/URANS, DNS, or quasi DNS approaches and apply a model of turbulence specially adapted for the melt turbulent flow computations. Advanced approximations of convective and diffusive terms allow the application of coarser computational grids and faster analysis. There are special tools for operative control of a computation.

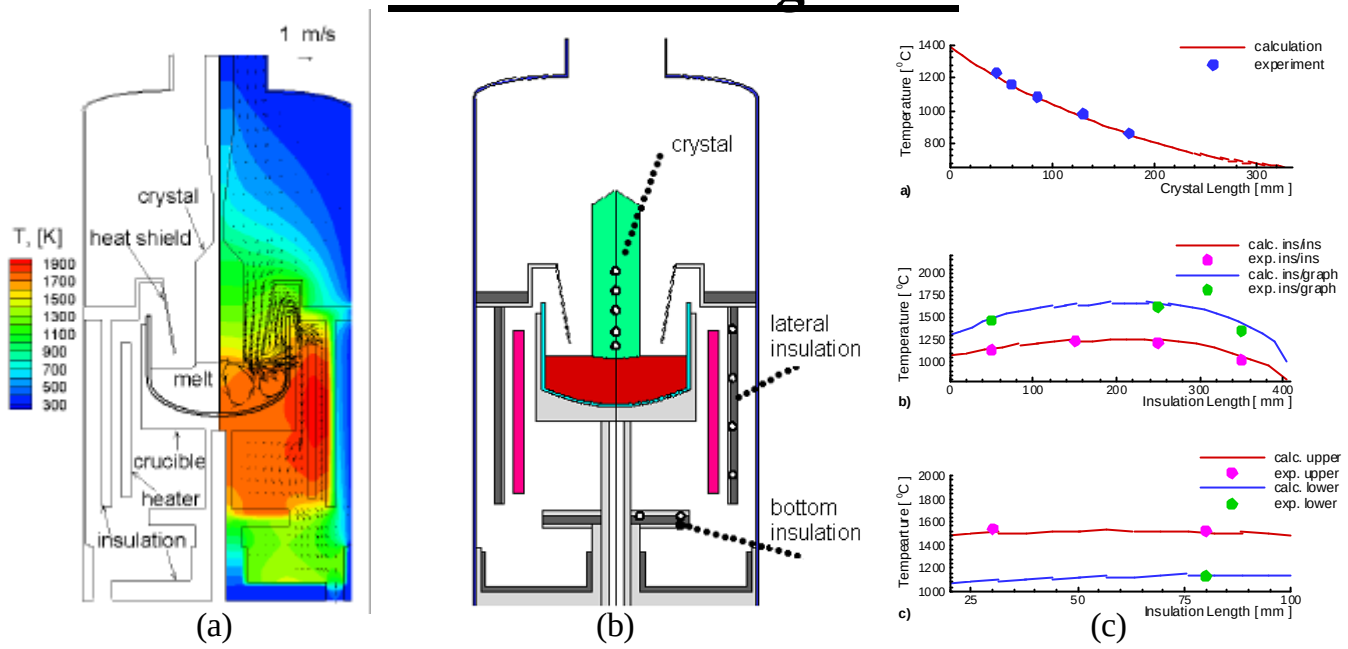


Flow Module accurately describes the geometry of the crystallization front, temperature gradients, distributions of velocity vectors and scalars, heat & mass fluxes along interfaces. There are options to analyze unsteady effects in several monitoring points and in cross sections of a 3D grid. Parallel version of the solver is also developed for using on Linux clusters or on several PCs in a Windows network.



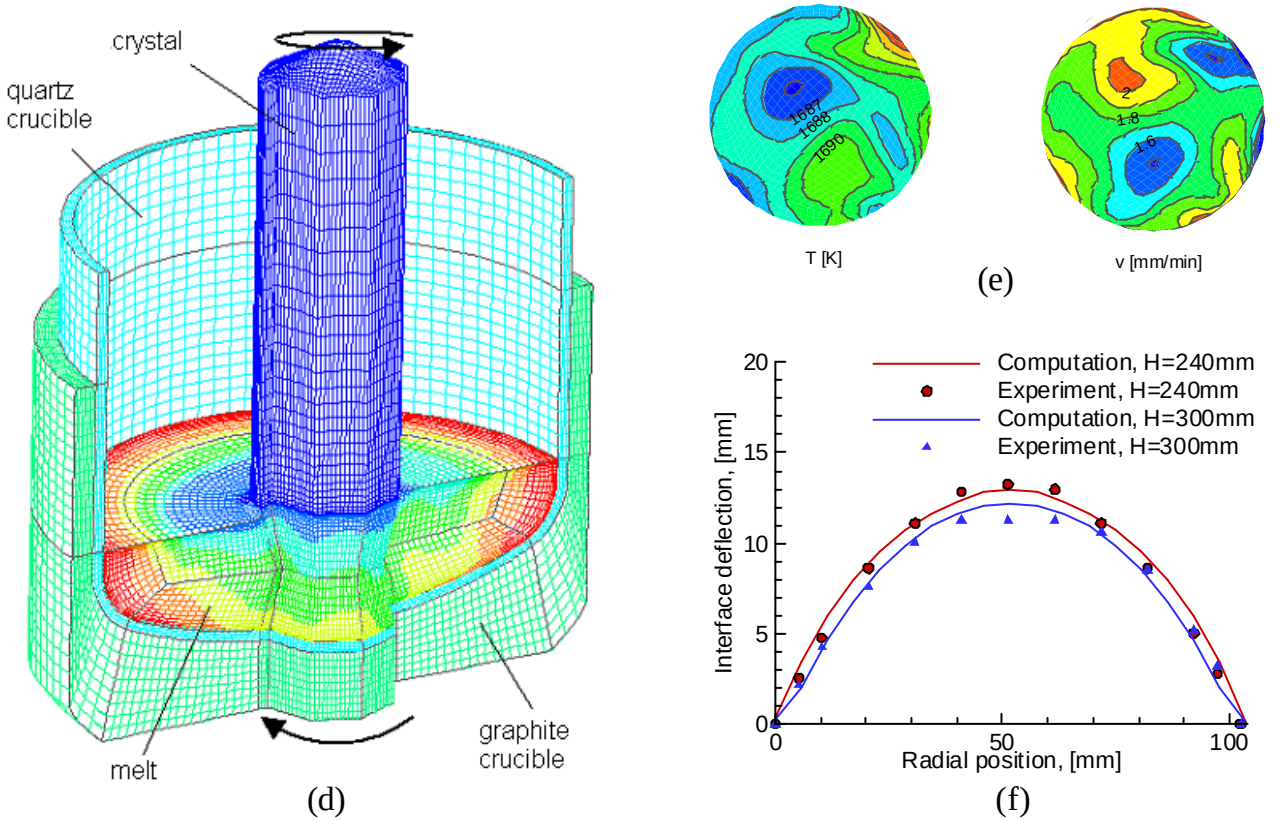
Examples of using *CGSim*

100 mm Si CZ growth



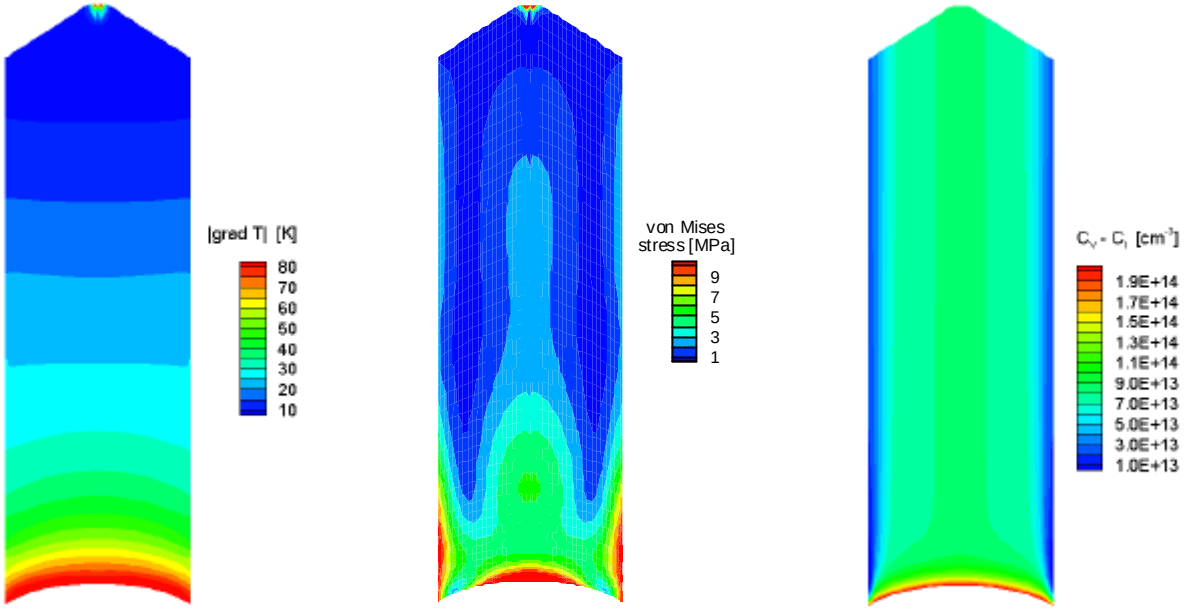
(a) (b) (c)

The furnace geometry and experimental data are published in J. Crystal Growth 180 (1997) pp. 461-467. The model of global heat transfer is presented in Refs. [1, 6]. The prediction of temperature distribution (a) is verified by comparing to experimental data (c) obtained in the points shown in (b). The computations demonstrate that the temperature is predicted very well if material properties are well known.



(d) (e) (f)

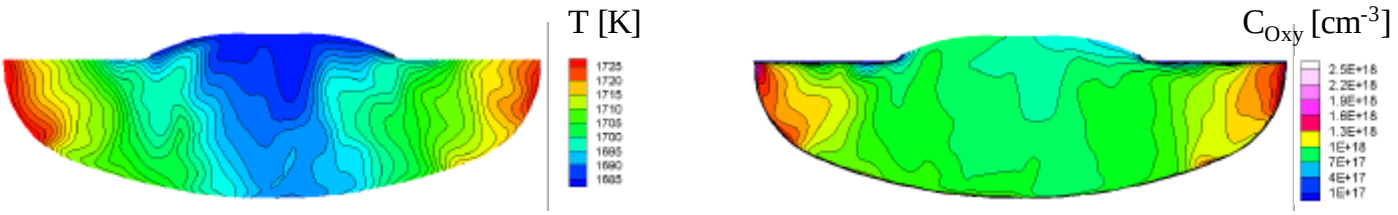
There is a 3D grid for the crystallization zone (d) including the melt, crucibles, and the crystal. ***Flow Module*** of ***CGSim*** was used to predict the geometry of the crystallization front (f) for the crystal heights of 240 and 300 mm [12, 18]. 3D unsteady behavior of melt flow results in strongly asymmetric instant distributions of the crystallization rate over the interface and the temperature under the crystal (e).



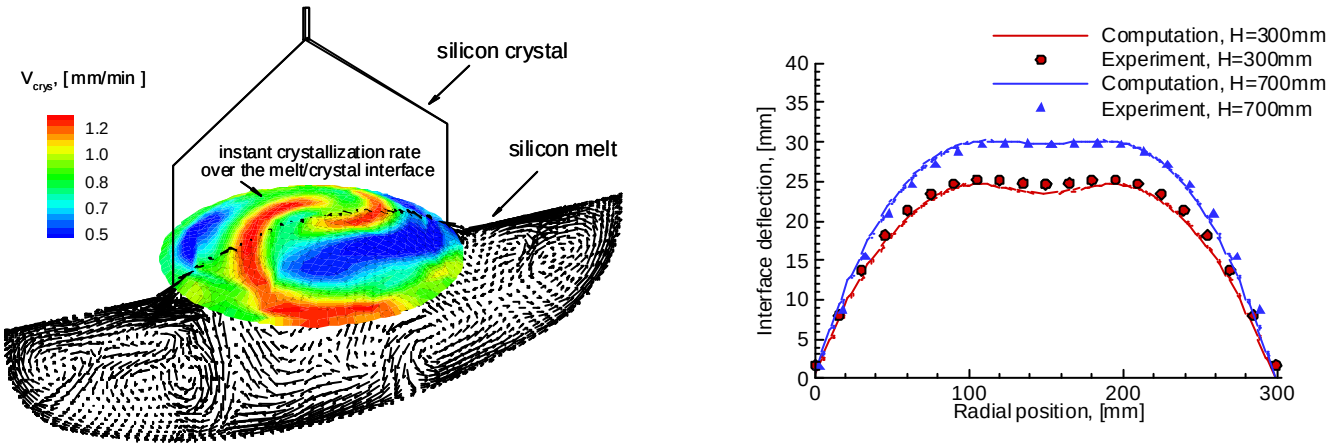
(g) (h) (i)

Accurate analysis of temperature gradients (g) and thermal stresses (h) is possible in Module ***"Defects"*** 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 (i) shows the type of dominating defects and the position of OSF ring.

300 mm Si CZ growth



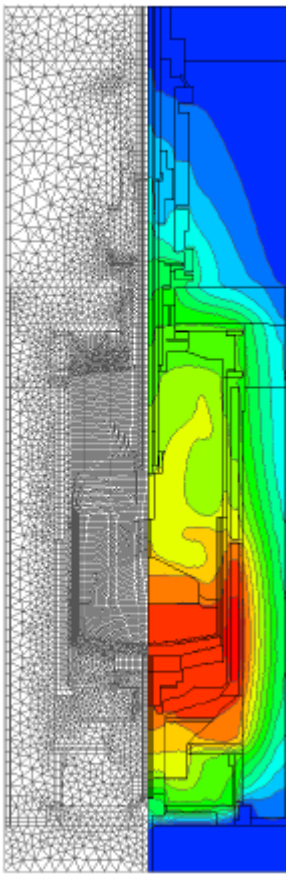
(a) (b)



(c) (d)

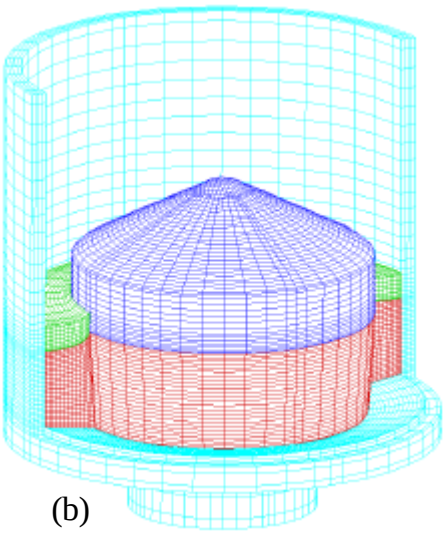
The effect of melt convection on the formation of the crystallization front is especially pronounced in the case of 300 mm Si growth. Heat (a) and mass transfer (b) is mostly governed by turbulent flow structures, which can be directly modeled in 3D unsteady analysis. The crystallization rate distribution over the crystallization front is strongly non-uniform and unsteady (c). Our 3D unsteady approach is successfully applied for industrial growth of 300 mm diameter crystals (d), see refs.[7, 18] for details.

VCz growth of 4 inch GaAs crystals

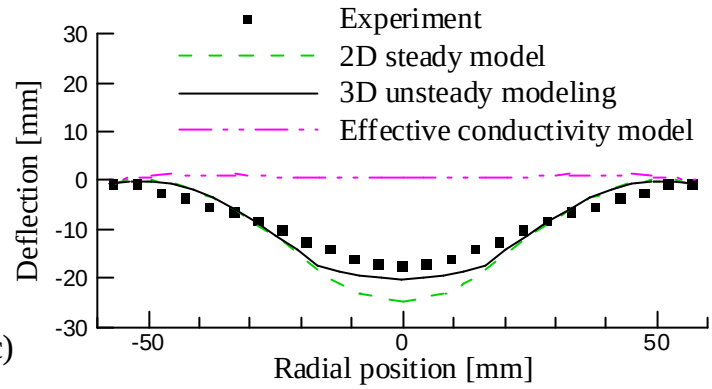


(a)

Numerical analysis of VCz and LEC growth is usually more complicated than the analysis of conventional CZ growth because of turbulent gas convection and the presence of encapsulant layer. ***CGSim*** software allows adequate consideration of all these phenomena (a) [10-11,13-14,19]. A 3D computational domain (b) is extended by including encapsulant flow. The geometry of the crystallization front predicted in computations is in a reasonable agreement with experimental data (c).

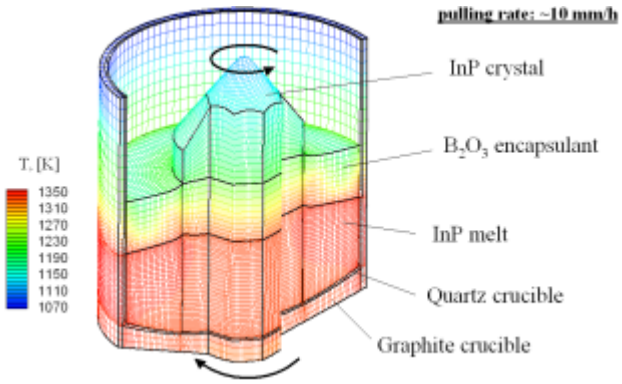


(b)



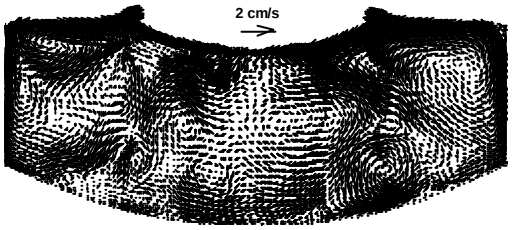
(c)

LEC growth of 4 inch InP crystals

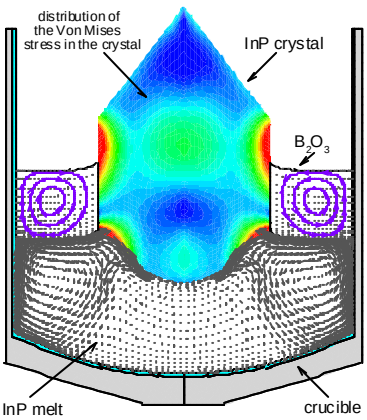


(a)

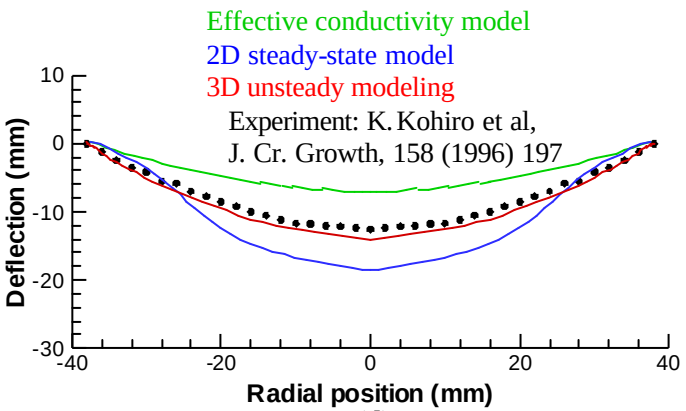
CGSim has also been shown as a powerful tool for analysis of LEC InP growth [9,13].



(b)

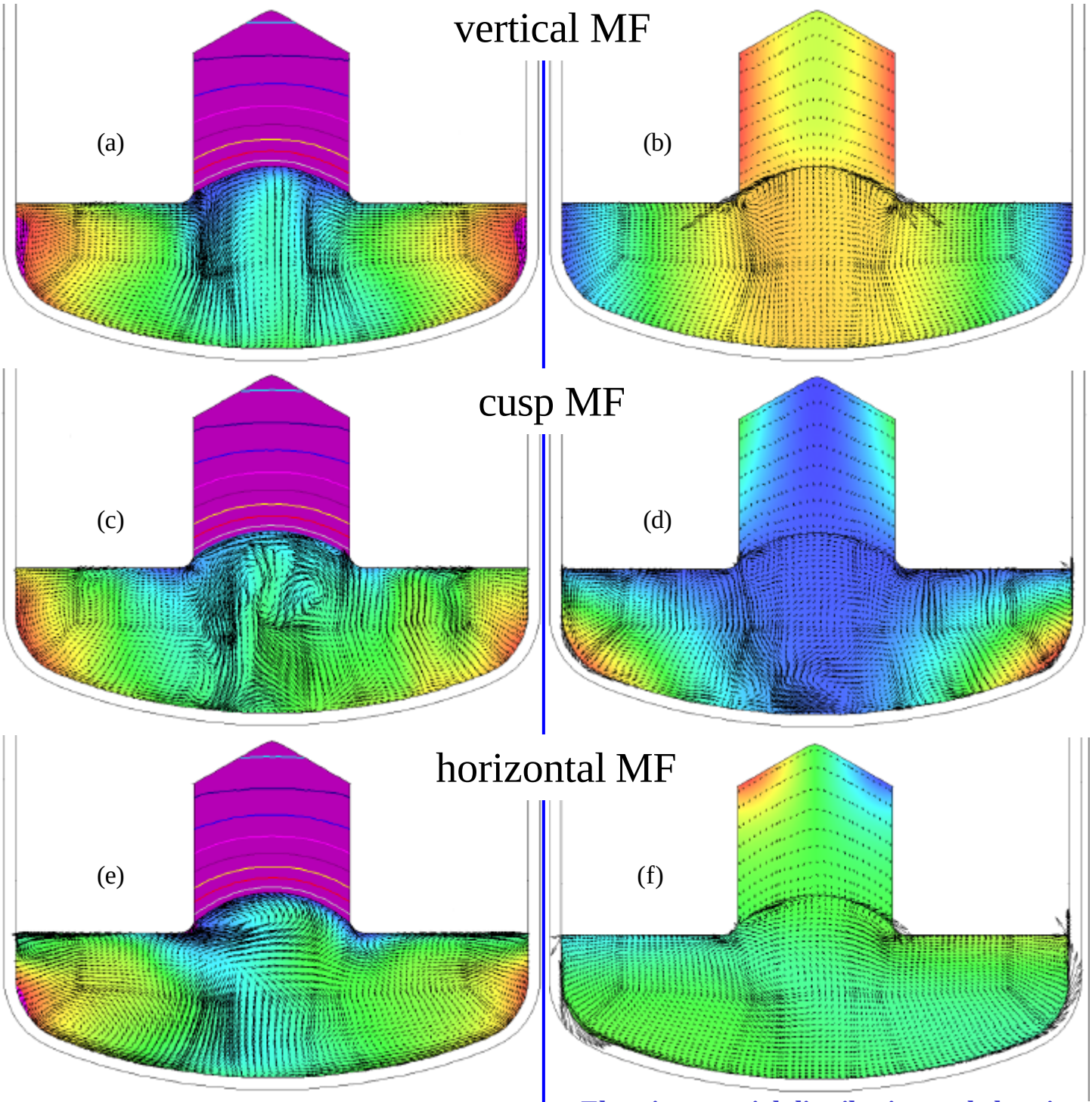


(c)



(d)

Effect of Magnetic Field on melt convection



Temperature distribution and velocity distribution in the melt (left).

Electric potential distribution and electric current flow in the melt and crystal (right).

Flow Module is extended by options for calculating magnetic field effects in the crystallization zone, including the conjugated electric current flow in the crystal and melt [8]. There are automatic options for direct current magnetic fields of uniform (vertical (a,b) / horizontal (e,f)) and cusp (c,d) configurations. Alternative current MFs can be implemented in a customized software version. Melt flow and the crystallization front can be analyzed in both 3D unsteady and 2D steady approaches. The examples of 3D unsteady modeling, presenting on this page, are provided for 100 mm Si CZ growth.

Selected references:

1. “Modelling analysis of oxygen transport during Czochralski growth of silicon crystals”, Yu.E. Egorov, Yu.N. Makarov, E.A. Rudinsky, E.M. Smirnov, A.I. Zhmakin, in: S.T. Dunham, J.S. Nelson (Eds.), Semiconductor Process and Device Performance Modelling, Mat. Res. Soc. Symp. Proc., vol.490, MRS, Pennsylvania, 1998, p.181.
2. “ Global model of Czochralski silicon growth to predict oxygen content and thermal fluctuations at the melt-crystal interface”, I.Yu. Evstratov, V.V. Kalaev, V.N. Nabokov, A.I. Zhmakin, Yu.N. Makarov, A.G.Abramov, N.G. Ivanov, E.A. Rudinsky, E.M. Smirnov, S.A. Lowry, E. Dornberger, J. Virbulis, E. Tomzig, W. v.Ammon, Microelectronic Engineering, 56/1-2 (2001) pp. 139-142.
3. “Modeling analysis of unsteady three-dimensional turbulent melt flow during Czochralski growth of Si crystals”, I.Yu. Evstratov, V.V. Kalaev, A.I. Zhmakin, Yu.N.Makarov, A.G. Abramov, N.G. Ivanov , E.M. Smirnov, E. Dornberger, J. Virbulis, E. Tomzig, W. v.Ammon, Journal of Crystal Growth 230 (2001) pp. 22-29.
4. “Modeling of impurity transport and point defect formation during Cz Si crystal growth”, V.V. Kalaev, V.A. Zabelin, Yu.N. Makarov, Solid State Phenomena 82-84 (2002) pp. 41-46.
5. "Numerical study of 3D unsteady melt convection during industrial-scale CZ Si-crystal growth", I.Yu. Evstratov, V.V. Kalaev, A.I. Zhmakin, Yu.N. Makarov,A.G. Abramov, N.G. Ivanov, A.B. Korsakov, E.M. Smirnov, E. Dornberger, J. Virbulis, E. Tomzig, W. von Ammon, Journal of Crystal Growth 237–239 (2002) 1757–1761.
6. “Gas flow effect on global heat transport and melt convection in Czochralski silicon growth”, V. V. Kalaev, I. Yu. Evstratov, Yu. N. Makarov, J. Crystal Growth, 249/1-2 (2003) pp. 87-99.
7. “Calculation of bulk defects in CZ Si growth: impact of melt turbulent fluctuations”, V.V. Kalaev, D.P. Lukanin, V.A. Zabelin, Yu.N. Makarov, J. Virbulis, E. Dornberger, W. von Ammon, J. Crystal Growth, 250/1-2 (2003) pp. 203-208.
8. “Analysis of magnetic field effect on 3D melt flow in CZ Si growth”, N.G. Ivanov, A.B. Korsakov, E.M. Smirnov, K.V. Khodosevitch, V.V. Kalaev, Yu.N. Makarov, E. Dornberger, J. Virbulis, W. von Ammon, J. Crystal Growth, 250/1-2 (2003) pp. 183-188.
9. “Prediction of the melt/crystal interface geometry in liquid encapsulated Czochralski growth of InP bulk crystals”, E.N. Bystrova, V.V. Kalaev, O.V. Smirnova, E.V. Yakovlev, Yu.N. Makarov, J. Crystal Growth, 250/1-2 (2003) pp. 189-194.
10. “Modeling analysis of vCZ growth of GaAs bulk crystals using 3D unsteady melt flow simulations”, E.V. Yakovlev, O.V. Smirnova, E.N. Bystrova, V.V. Kalaev, Ch. Frank-Rotsch, M. Neubert, P. Rudolph, Yu.N. Makarov, J. Crystal Growth, 250/1-2 (2003) pp. 195-202.
11. “Global heat and mass transfer in vapor pressure controlled Czochralski growth of GaAs crystals”, E.V. Yakovlev, V.V. Kalaev, I.Yu. Evstratov, Ch. Frank, M. Neubert, P. Rudolph, Yu.N. Makarov, J. Crystal Growth, 252/1-3 (2003) pp. 26-36.
12. “Prediction of bulk defects in CZ Si crystals using 3D unsteady calculations of melt convection”, V.V. Kalaev, D.P. Lukanin, V.A. Zabelin, Yu.N. Makarov, J. Virbulis, E. Dornberger, W. von Ammon, Materials Science in Semiconductor Processing, 5/4-5 (2003) pp. 369-373.
13. “Modeling Analysis of Liquid Encapsulated Czochralski Growth of GaAs and InP Crystals”, E.V.Yakovlev, V.V. Kalaev, E.N. Bystrova, O.V. Smirnova, Yu.N. Makarov, Ch. Frank-Rotsch, M. Neubert, P. Rudolph, Crystal Research and Technology, 38, No. 6 (2003) pp. 506-514.
14. “3D unsteady numerical analysis of conjugate heat transport and turbulent/laminar flows in LEC growth of GaAs crystals”, O.V. Smirnova and V.V. Kalaev, International Journal of Heat and Mass Transfer 47 (2004) pp. 363-371.
15. “Modeling of point defect formation in silicon monocrystals”, V. A. Zabelin and V. V. Kalaev, Microelectronic Engineering 69 (2003) pp. 641-645.
16. “Variations of solid–liquid interface in the BGO low thermal gradients Cz growth for diffuse and specular crystal side surface”, V.S. Yuferev, O.N. Budenkova, M.G. Vasiliev, S.A. Rukolaine, V.N. Shlegel, Ya.V. Vasiliev, A.I. Zhmakin, J. Crystal Growth 253 (2003) 383–397.
17. “Parallel Simulation of Czochralski crystal growth”, D. Lukanin, V. Kalaev, A. Zhmakin, Lecture Notes in Computer Science, Vol. 3019 (2004) pp. 469–474.
18. “Advances in the simulation of heat transfer and prediction of the melt-crystal interface shape in silicon CZ growth”, D.P. Lukanin, V.V. Kalaev, Yu. N. Makarov, T. Wetzel, J. Virbulis, and W. von Ammon, J. Crystal Growth, 266/1-3 (2004) pp. 20–27.
19. “3D Computations of Melt Convection and Crystallization Front Geometry during VCz GaAs Growth” O.V. Smirnova, V.V. Kalaev, Yu.N. Makarov, Ch. Frank-Rotsch, M. Neubert, P. Rudolph, J. Crystal Growth 266 (2004) pp 67–73.
20. “Simulation of Heat Transfer and Melt Flow in Czochralski Growth of Si1-xGex Crystals”, O.V. Smirnova, V.V. Kalaev, Yu.N. Makarov, N.V. Abrosimov, H. Riemann, J. Crystal Growth 266 (2004) pp. 74–80.