Finansējuma saņēmēja nosaukums
Latvijas Universitāte

Īstenotā projekta nosaukums
„Jaunas matemātiskās modelēšanas instrumentu sistēmas izstrāde funkcionālo nano- un mikroelektronikas pusvadītāju materiālu ražošanas tehnoloģijām"

Īstenotā projekta Nr.
2011/0002/2DP/2.1.1.1.0/10/APIA/VIAA/085

Projekta LU reģistrācijas Nr.
ESS2011/121

Projekta zinātniskais vadītājs
Dr.-Phys., asoc. prof. Andris Muižnieks

Atskaite par periodu 01.07.2011. – 30.09.2011.

Projekta ietvaros plānots izveidot papildinājumu ar nanomērogu, kinētiskiem un mikroskopiskiem modeļiem matemātiskās modelēšanas un programmu bāzes sistēmai (MMPBS), kas tiek izmantota funkcionālo un pusvadītāju materiālu ražošanas tehnoloģiju matemātiskajā modelēšanā un kas ir izstrādāta un implementēta programmu kompleksa veidā uz Fizikas un Matemātikas Fakultātes daudzprocesoru klastera. Tas ļaus analizēt gan tehnoloģisko procesu makroskopiskos, gan nanomērogu, kinētiskos un mikroskopiskos procesus, gan to saistību.

1. Konferences un semināri

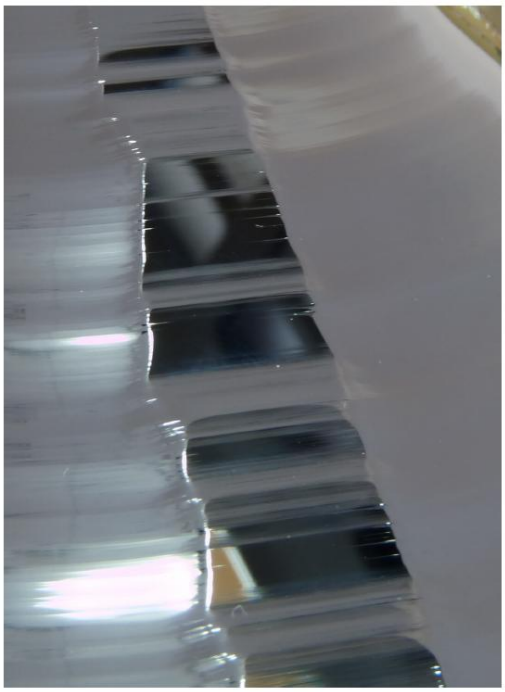
Pārskata periodā tika sagatavoti, iesniegti un pieņemti 4 referāti (katram 1 lpp. tēzes, kas tiks izdotas tēžu rājumā) starptautiskam seminārам *Workshop "Multiphysical Modelling in OpenFOAM"*, kas notiks Rīgā 2011. g. 20. un 21. oktobrī un ko organizē *Institute of Electrotechnology, Leibniz University of Hanover (Hanover, Germany)* un Vides un Tehnoloģisko Procesu Matemātiskās Modelēšanas Laboratorija (Latvijas Universitāte, Fizikas un Matemātikas Fakultāte).

Referātu autori un nosaukumi ir sekojoši:

1. Andrejs Sabanskis, Andris Muiznieks, Armands Krauze. *Modeling of Argon flow in FZ silicon single crystal growth system using OpenFOAM.*
2. Armands Krauze, Andris Muiznieks, Normunds Jekabsons. *Modeling of turbulent melt flow in CZ silicon single crystal growth system using OpenFOAM.*
3. Kārlis Janiselis, Andris Muižnieks, Kaspars Lācis. *Modeling of melt flow in FZ silicon single crystal growth system using OpenFOAM.*
4. Kristaps Bergfelds, Andris Muižnieks, Armands Krauze. *Silicon melting in could crucible heated with electron beam; modeling using OpenFOAM.*

2. Komandējumi

Pārskata periodā projekta zinātniskais vadītājs Andris Muižnieks komandējumā laikā no 10.07.2011. līdz 14.07.2011. apmeklēja silīcija monokristālu audzēšanas firmu *Siltronic AG, Burghausen,* Vācija 10. 14. 07. 2011. Šī komandējuma laikā tika iegūti eksperimentālie dati par kristalogrāfiski noteiktu šķautņu veidošanos uz kristālu virsmas dažādos kristālu audzēšanas apstākļos, ilustrācijai skatīt nelielu fragmentu no iegūtajiem datiem attēlā zemāk.



Šie dati tiks izmantoti, lai pārbaudītu izstrādājamos nanomērogu, kinētiskos un mikroskopiskos modeļus, kuri veidos bāzi projekta mērķim – „Jaunas matemātiskās modelēšanas instrumentu sistēmas izstrāde funkcionālo nano- un mikroelektronikas pusvadītāju materiālu ražošanas tehnoloģijām".

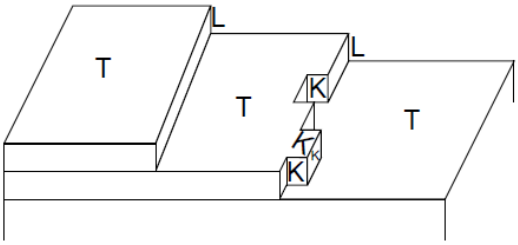
3. Literatūras analīze

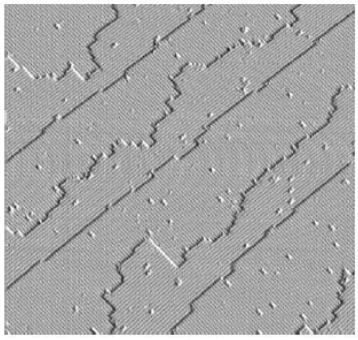
Līdz šī projekta sākumam bija izveidota matemātiskās modelēšanas un programmu bāzes sistēma (MMPBS), kas tika izmantota funkcionālo un pusvadītāju materiālu ražošanas tehnoloģiju matemātiskajā modelēšanā. Šī sistēma raksturojās ar to, ka tehnoloģiskie procesi tika aprakstīti izmantojot makroskopiskos modeļus. Lai uzsāktu nanomērogu, kinētisko un mikroskopisko modeļu izstrādi, tika veiktas apjomīgas literatūras studijas. Zemāk norādām dažus no svarīgākajiem avotiem.

1. G.F. Bolling, W.A. Tiller, "Growth from the Melt. I. Influence of Surface Intersections in Pure Metals", J Appl. Phys. 31, 1345 (1960).
2. V. V. Voronkov. "Mass transfer at the surface of a crystal near to its boundary with the melt, and its influence on the shape of the growing crystal", Kristallografiya 23, 249 (1978).
3. M. Elena Diaz, Javier Fuentes, Ramon L. Cerro, Michael D. Savage, "Hysteresis during contact angles measurement", Journal of Colloid and Interface Science 343, 574 (2010).
4. Crystal Growth Processes Based on Capillarity. Edited by T. Duffar (2010).

5. D.J. Eaglesham, A.E.White, L.C. Feldmann, N. Moriya, D.C. Jacobson, "Equilibrium shape of Si", Phys. Rev. Lett. 70 (1993) 1643.
6. Apte and Zeng "Anisotropy of crystalmelt interfacial free energy of silicon by simulation", Appl. Phys. Lett 92, 221903 (2008).
7. V. V. Voronkov. "Theory of crystal surface formation in the pulling process", Journal of Crystal Growth 52 311 (1981).

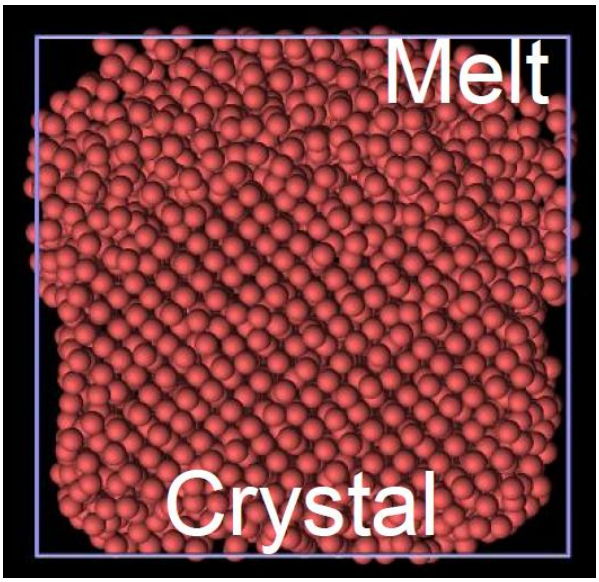
Galvenie fizikālie aspekti, kas tika pētīti literatūras studijās ir gan termodinamisko fāzu robežu apraksts, izmantojot *Gibbs-Thomson* vienādojumu, gan kinētiskais modelis *Terrace Ledge Kink (TLK)*, kas apraksta virsmas evolūciju, lietojot virsmas defektu formēšanos (terases, pakāpieni, izvirzījumi), skatīt attēlu zemāk, gan šo abu pieeju saistība.





4. Molekulārās dinamikas metodes lietošana

Lai aprakstītu fāzu pārejas atomu mērogā, tika instalēta atvērtā koda programmu pakete LAMMPS, kas ļauj veikt aprēķinus, izmantojot molekulārās dinamikas metodi. Pakete LAMMPS ir instalēta uz 4 procesoru darba stacijas ar operāciju sistēmu *ubuntu 11.04*. Ir veikti pirmie aprēķini silīcija kristāliskai un izkusušajai fāzēm un fāzu robežai starp tām, aprēķinu rezultātu ilustrācijai skatīt attēlu zemāk.



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5. Atvērtā koda paketes hidrodinamisko aprēķinu veikšanai OpenFOAM pielietošana silīcija kristālu audzēšanas procesu matemātiskajai modelēšanai

Tika veikts būtisks darbs, lai adaptētu un pielietotu atvērtā koda paketi OpenFOAM, kas ir paredzēta trīsdimensionālu hidrodinamisku aprēķinu veikšanai, silīcija monokristālu audzēšanas procesu matemātiskajā modelēšanā. Šādas makroskopiskas modelēšanas rezultāti kalpos kā ieejas informācija mikroskopisku aspektu modelēšanā. Būtiskākie šie darba rezultāti ir pieteikti kā referāti iepriekš minētajā starptautiskajā seminārā *Workshop "Multiphysical Modelling in OpenFOAM"*. Tāpēc tālāk šīs atskaites tekstā kā sadaļas iekļaujam pieteiktos referātu abstraktus.

5.1. Modeling of argon flow in FZ silicon single crystal growth system using OpenFOAM

Andrejs Sabanskis, Andris Muiznieks, Armands Krauze
University of Latvia, Faculty of Physics and Mathematics

The mathematical modeling is now widely established as one of development instruments for the industrial silicon single crystal floating zone (FZ) growth for electronic needs. The corresponding system of mathematical models includes temperature and velocity fields in the melt, the mass transport of impurities and dopants, heat exchange via radiation in the whole system, the use of electromagnetic fields for silicon melting and for the control of the melt motion, the segregation process at the crystallization front etc., see, e.g., [1,2].

Nowadays the development of the FZ process is headed for the growth of large-diameter (up to 200 mm) crystals. It is experimentally observed that for large crystals the convection of argon (Ar) atmosphere becomes more pronounced and has larger influence on the FZ process. Typical pressure of Ar is 1-2 atm, and it is necessary to avoid the electric breakdown at the high-frequency inductor (typical voltage – 1000 V). Due to larger influence of Ar convection, thermal boundary layers are more pronounced, which results in larger temperature gradients at the silicon surface. The heat flux density, transferred by Ar, can become comparable to the radiation heat flux density; therefore it has to be taken into account. Since the highest temperature in the system is about 1700 K (melt) and the lowest about 400 K (water cooled metallic parts), the Ar density in the vessel varies about 4 times, i.e., the Boussinesq approximation cannot be used [3]. The characteristic velocities in the system are much lower than the speed of sound; nevertheless, a turbulent flow regime is expected.

For the modeling of the Ar flow in FZ setup, the solver *buoyantSimpleFoam* from open source library *OpenFOAM 2.0.1* is used, which allows describing the essential density changes. The gas is modeled as an ideal gas, using the SST k-omega turbulence model. Because the considered 3D solver is used for axisymmetric flow, the grid is generated with one layer in azimuthal direction and the *wedge* boundary conditions are used. The additional cooling of the crystal due to Ar flow is investigated and compared with the heat radiation. An example of calculated Ar flow is shown below: in the left figure finite volume mesh and turbulent viscosity are depicted, figure on the right shows temperature and velocity fields.

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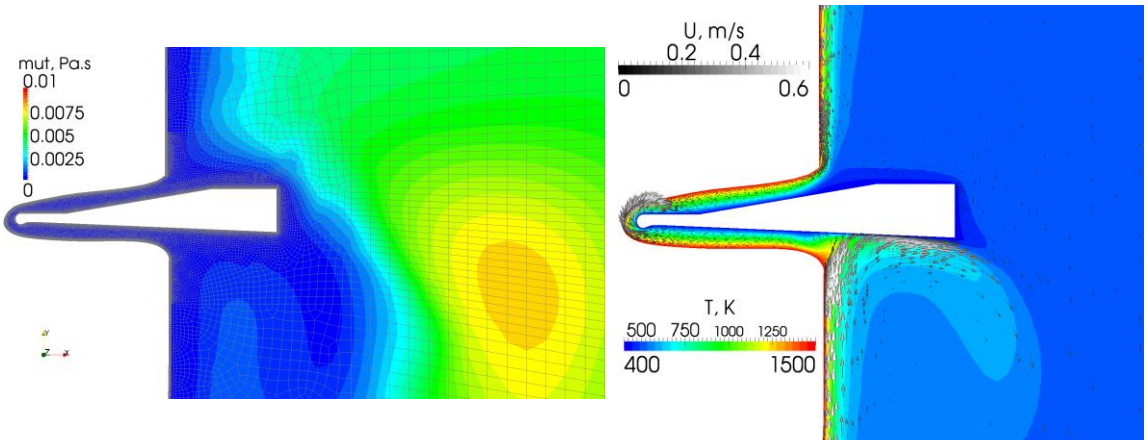

Acknowledgements
The present work is carried out at the University of Latvia and has been supported by the European Regional Development Fund, project contract No. 2011/0002/2DP/2.1.1.1.0/10/APIA/VIAA/085 and by the European Social Fund, project contract No. 2009/0223/1DP/1.1.1.2.0/09/APIA/VIAA/008 and within the project "Support for Doctoral Studies at University of Latvia".

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1. A. Krauze, N. Jēkabsons, A. Muižnieks, A. Sabanskis, and U. Lācis. Applicability of LES turbulence modeling for CZ silicon crystal growth systems with traveling magnetic field. *Journal of Crystal Growth*, 312(21):3225–3234, 2010.
2. K. Lācis, A. Muižnieks, A. Rudevičs, and A. Sabanskis. Influence of DC and AC magnetic fields on melt motion in FZ large Si crystal growth. *Magnetohydrodynamics*, 46(2):199–218, 2010.
3. V.V. Kalaev, I.Yu. Evstratov, and Yu.N. Makarov. Gas flow effect on global heat transport and melt convection in Czochralski silicon growth, *Journal of Crystal Growth*, 249(1-2):87-99, 2003.

5.2. Modelling of turbulent melt flow in CZ silicon single crystal growth system using OpenFOAM

Armands Krauze[1], Andris Muiznieks[1], Normunds Jekabsons[2]
1) University of Latvia, Faculty of Physics and Mathematics; 2) Ventspils University College

Mathematical modelling of the melt flow and heat transfer for industrial Czochralski (CZ) Si single crystal growth systems has become an important instrument for optimization of the crystal growth processes. Open-source program package *OpenFOAM* is a set of HD and heat transfer solvers and pre- and post-processing tools that after proper adaptation can be used to model almost every aspect of the industrial Si crystal growth. *OpenFOAM* is extremely flexible and allows the user to create new tools, solvers, and boundary conditions to suit their needs. It comes also with a large set of built-in turbulence models and provides means for parallelization of calculations.

The modern industrial CZ Si crystal growth systems are characterized by high-Re (about 10^5) 3D melt flows which necessitates modelling turbulence effects. In our calculations, we have used the *OpenFOAM* Smagorinsky-Lilly LES model for an incompressible fluid with van Driest turbulence damping at solid walls and constant melt quantities [1]. The buoyancy forces were modelled in Boussinesq approximation. The

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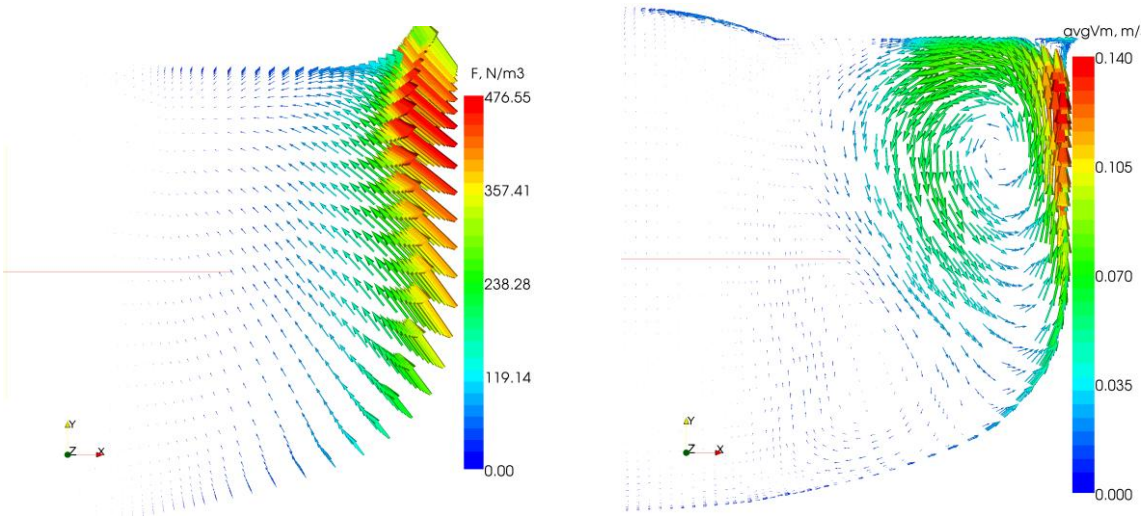
calculations results from a 2D axisymmetric heat transfer modelling for the whole system, e.g. [2], were used for the temperature calculation in the melt as boundary conditions.

In the present work, the influence of different axisymmetric travelling EM fields on the melt flow was examined. The EM force density field in the melt was calculated by a 2D axisymmetric electromagnetic (EM) field model and interpolated for a 3D mesh for the HD calculations. To use EM volume forces in the melt flow modelling, we have developed a special *OpenFOAM* solver *czlesfoam*. Calculations were performed on several grids, with the finest grid having 242041 cells. The calculations had to be run by about 2000 s of the flow time, before the flow more or less stabilized. After that the melt flow and temperature fields were averaged for 100 s of the flow time. Below an example of calculations is shown for the influence of an upwards-driving travelling field on the Si melt flow (left – EM force density, right – velocity field).



Acknowledgements
The present work is carried out at the University of Latvia and at the Ventspils University College and has been supported by the European Regional Development Fund, project contract No. 2011/0002/2DP/2.1.1.1.0/10/APIA/VIAA/085, and by the European Social Fund, project contracts: No. 2009/0223/1DP/1.1.1.2.0/09/APIA/VIAA/008 and No. 2009/0231/1DP/1.1.1.2.0/09/APIA/VIAA/151.

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1. A. Krauze, N. Jēkabsons, A. Muižnieks, A. Sabanskis, and U. Lācis. Applicability of LES turbulence modeling for CZ silicon crystal growth systems with traveling magnetic field. *Journal of Crystal Growth*, 312(21):3225–3234, 2010.
2. V.V. Kalaev, I.Yu. Evstratov, and Yu.N. Makarov. Gas flow effect on global heat transport and melt convection in Czochralski silicon growth, *Journal of Crystal Growth*, 249(1-2):87-99, 2003.

5.3. Silicon melting in cold crucible heated with electron beam; modeling using OpenFOAM

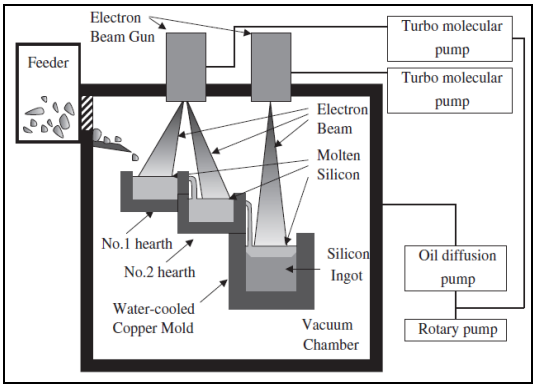
Kristaps Bergfelds[1], Andris Muižnieks[2], Armands Krauze[2]
1) Institute of Solid State Physics, University of Latvia 2) University of Latvia, Faculty of Physics and Mathematics

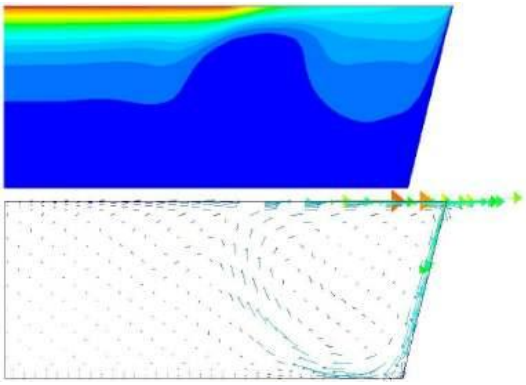
Because of the needs of the photovoltaic power industry, intensive research is carried out nowadays for the development of economical mass production methods for producing solar-grade silicon (SOG-Si) from metallurgical-grade silicon (MG-Si).

One of such methods is the melting and purifying of MG-Si in a water-cooled copper crucible by using electron beam technology [1]. Polycrystalline silicon in a crucible is melted by an electron beam which is directed vertically downwards to the free surface of silicon. High overheating temperatures (several hundreds of degrees) ensure effective evaporation of some impurities. In this way silicon could be purified relatively cheaply and in large quantities. Because of extremely high temperature gradients in the silicon, the process must be controlled with great precision. Therefore it is important to develop adequate mathematical models which describe melt motion, temperature field in the molten silicon and solid silicon layers at the crucible wall.

In the present work, several axisymmetric mathematical models are proposed for the modeling of the considered system. The solid silicon layers at the crucible wall are analyzed with *FEMM* package; the turbulent melt flow is modeled using *ANSYS FLUENT*. The melt flow was also modeled with solver *buoyantBoussinesqSimpleFoam* from open source library *OpenFOAM 2.0.1*., and SST k-omega turbulence model were used. In general the *OpenFOAM* solvers are based on the 3D modeling of fluid flow. Therefore for axisymmetric calculations, a 3D grid is generated with one cell layer in the azimuthal direction, and the *wedge* boundary condition is used.

In the figure below (left), a general scheme of the silicon purifying system by using electron beams (picture from [1]) is shown on the left. On the right an example of calculations of melt motion in the cold crucible is shown: top - temperature distribution; bottom – velocity distribution.





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1. Kazuhiro Hanazawa, Noriyoshi Yuge, Yoshiei Kato. Evaporation of Phosphorus in Molten Silicon by an Electron Beam Irradiation Method. *Materials Transactions*, Vol. 45, No. 3 (2004) pp. 844 to 849.

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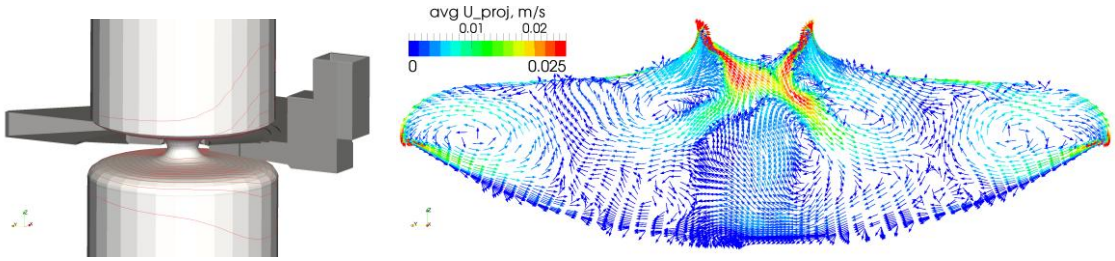
5.4. Modeling of melt flow in FZ silicon single crystal growth system using OpenFOAM

Kārlis Janiselis, Andris Muižnieks, Kaspars Lācis.
University of Latvia, Faculty of Physics and Mathematics

The continuous development of the Si single crystal growth industry requires the enhancement of both the product quality and the production speed. As the laboratory experiments of floating zone (FZ) Si single crystal growth process are very expensive, numerical modeling is frequently used to simulate the process. One of the main desired results from numerical modeling is calculated distribution of resistivity in the grown crystal. The resistivity is directly influenced by distribution of dopants in the melt, which can be obtained only by coupled calculation of melt motion and dopant transport. Numerical and experimental results were compared in [1], however these calculations were performed in 2D axis-symmetric approach. We present the new comparison of experimentally measured resistivity profiles in the Leibniz Institute for Crystal Growth (Berlin) and calculated profiles obtained from unsteady 3D calculations of 100mm Si single crystal growth process by FZ method.

The whole calculation cycle includes 2D axis-symmetric calculation of phase boundaries (taking into account the pull and rotation rates), 3D calculation of HF EM field in the system (see half of the HF inductor and calculated eddy currents on the surface of silicon in the figure below on the left) and 3D unsteady calculations of melt motion, temperature field and dopant transport in molten silicon. The complete system of used mathematical models is described in [2].

The HD calculations were performed with our solver *fzFOAM* for modeling of FZ process which is based on open source library *OpenFOAM*. For the calculations a block-structured hexahedral mesh with 150000 elements and time step 0.5 ms were used. An example of calculated velocity distribution in the melt in the vertical cross-section is shown in the figure below on the right. During the calculations one of the most uncertain parameters was the thermal gradient of surface tension or so called Marangoni coefficient, which can vary in a certain range depending on the atmosphere content in the vessel and other factors. As the first calculations of melt motion were performed with Marangoni coefficient Ma=-0.00025 N/(m·K), additional calculations with different values were performed with the goal to match the number and the positions of the minimums of the normalized resistivity. The best correspondence of numerical and experimental results was achieved with Ma=-0.00013 N/(m·K).



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[2] K. Lacis, A. Muiznieks, A. Rudevics, A. Sabanskis. Influence of DC and AC magnetic fields on melt motion in FZ large Si crystal growth. Magnetohdrodynamics, Vol. 46 (2010), No. 2, pp. 199-218.

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