Numerical Aspects of Modelling of Coil System for Rotating Magnetic Field

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Abstract

The paper analyses the precision of the calculation results of low frequency rotating magnetic field and corresponding force density distribution in the melt domain of a 4" floating zone crystal growth system. The magnetic fields in such systems due to technical reasons often are extremely inhomogeneous. For the calculations an edge finite element method based specialized self-developed software is used. Influence of the numerical parameters of calculation, such as pre-conditioners, admissible tolerance value and the mesh density, on the obtained results is examined.

Introduction

The rotating magnetic field (RMF) is often used in various industrial processes where additional stirring of conductive melts is necessary. The use of RMF is of great interest also in semiconductor crystal growth processes, where contact-free interaction with melt is essentially important due to the necessary purity of the grown crystal. Therefore in last years the experimental work and calculations are intensively discussed in literature. For example, Y. Gelfgat et. al. in [1] have carried out simulations to determine the effect of various rotating electromagnetic field configuration parameters on magnetohydrodynamic melt flow structure and velocity distributions in a cylindrical vessel. Experimental studies have shown that in Czochralski crystal growth system a flow transition from large scale buoyancy driven to small scale magnetically driven turbulence occurs in the presence of RMF [2]. P. Dold et. al. in [3] have experimentally shown that application of RMF in Floating Zone (FZ) silicon crystal growth reduces dopant fluctuations caused by time dependent thermocapillary convection. Numerical results in [4] also show that both – axial and radial segregation process can be homogenized with application of RMF in vertical gradient freeze growth of Ge crystals. Possibilities to control the radial melt motion along the crystallization interface in FZ process with needle-eye induction coil with applied RMF are shown in [5].

However publications rarely address the problem that the source of the RMF, i.e. the coils, due to technical reasons is usually positioned relatively far from the domain with the melt which has to be influenced. Consequently the magnitude of the so called stray field in the analyzed domain is much smaller than in the vicinity coils. The numerical simulation of such strongly inhomogeneous field demands thorough analysis of used parameters of numerical calculation procedure and the density of meshes. The present paper analyses the precision of the calculation results of magnetic field and corresponding force density distribution in the melt domain of a 4" FZ crystal growth system with RMF. For the calculations an edge finite element method (FEM) based specialized self-developed software *EM3D* [6] is used.

1. Description of Calculation Method and of the Considered System

EM3D [6] is a self-developed finite element program for calculating of threedimensional low-frequency magnetic fields using magnetic vector potential and electric scalar potential formulation. The program calculates besides the magnetic field and current density vectors also force density distribution. For the preparation of geometry of calculated system and for the generation of 3D finite element mesh, several program packages can be used, e.g., the commercial program package *Gambit*. The numerical aspects of used FEM are described in [6]. The solution process is iterative and it is controlled by: 1) tolerance criterion; 2) the maximal iteration count which determines the number of iterations which are performed if the desired tolerance criterion is not met. Two possible pre-conditioners for the solver: ILU and ILUT can be specified. ILU stands for incomplete LU factorization, while ILUT denotes incomplete Cholesky factorization and requires less computer memory for storing of the coefficient matrix. Number of the solutions of last iterations which are kept in memory for the calculation of the next iteration can also be set. The decrease of this number reduces the RAM memory necessary for the calculation; however, it also decreases the speed of the calculations and obtaining the convergent solution.

The considered electromagnetic system for rotating magnetic field is shown in Fig. 1. The system has three distinct domains – atmosphere (e.g., argon), melt and inductors. The inductors are actually cylindrical coils with defined current density. The electric conductivity of considered melt (silicon) is $1.2 \cdot 10^6$ S/m and of atmosphere is 0. The AC field frequency f = 50 Hz is used for all calculations. The rotating field in the melt is obtained by switching coils to three-phase current. As a boundary condition for the outer system surface, the condition that the magnetic field has only tangential component is used. The distance between symmetry axis of the melt and the inductors is 11 cm. For the calculations three finite element meshes were generated: rough mesh (178 000 tetrahedrons), the so called base mesh (341 000 tetrahedrons) and fine mesh (604 000 tetrahedrons).



Fig. 1. Left - system geometry with the finite element mesh (base mesh) with 341 000 tetrahedrons. Right – calculated real part of the magnetic field in the base mesh; side view of the vertical cross-section (*xz* plane); constant length vectors; magnetic field scale T; ILUT preconditioning; final residual value $2.7 \cdot 10^{-10}$

2. Calculation Results

2.1. Calculation Results Obtained with the Base Mesh

For the calculations with the base mesh the ILUT pre-conditioner is used. Final residual of EM field calculation is $2.7 \cdot 10^{-10}$. The obtained results are shown in Figs. 1-3.



Fig. 2. Magnetic field in the melt. Top left – real part, top view; top right – imaginary part, top view; bottom – real part, side view. Constant length vectors; magnetic field scale in T. The base mesh



Fig. 3. Force density distribution in the melt. Top view. Constant length vectors; force density scale in N/m^3 . The base mesh

Comparing the magnitude of the magnetic field in the coils (Fig. 1) and in the melt (Fig. 2) the obtained ratio is roughly 200. The characteristic value of the magnetic field in the melt is $3.5 \cdot 10^{-5}$ T = 0.035 mT = 35 μ T. As the direction of the magnetic field is rotating in time, the consequent averaged force density is directed azimuthally, see Fig. 3.

2.2. Calculation Results Obtained with the Fine Mesh

The knowledge of the concrete value of the magnetic field in the melt is very important, therefore the calculations have to be thoroughly verified as the magnitude in the melt is <1% than the maximal observed value in the calculated domain. To clear this, the current subsection presents the results of calculations for the system with refined mesh consisting of approximately 604 000 tetrahedrons.

If the ILUT pre-conditioner is used, the residual of EM field calculation after 80 iterations is $2.0 \cdot 10^{-5}$, after 120 iterations it is $9.0 \cdot 10^{-7}$, but then the convergence process dramatically slows down and after 2000 iterations the final residual is only $8.0 \cdot 10^{-7}$. Fig. 4 shows that the obtained solution is not converged since the magnetic field does not have the expected distribution in the melt. It can be explained by the fact that the magnetic field in the region of the melt is only a so called stray field and the given solution parameters disallow to obtain converged solution.



Fig. 4. Real part of the magnetic field in the system. Side view of the vertical cross-section (xz plane). Constant length vectors; magnetic field scale in T. System with refined mesh. ILUT pre-conditioner, final residual $8.0 \cdot 10^{-7}$

Change of the pre-conditioner from ILUT to ILU leads to final residual $2.5 \cdot 10^{-12}$ of EM field calculation. The obvious influence on the results can be seen in Fig. 5. The characteristic magnetic field and force density values are the same as in the case with base mesh (the maximal difference is about 1%).



Fig. 5. Real part of the magnetic field in the system. Side view of the vertical cross-section (xz plane). Constant length vectors; magnetic field scale in T. System with refined mesh. ILU preconditioner, final residual $2.5 \cdot 10^{-12}$

2.3. Calculation Results Obtained with the Rough Mesh

The current subsection presents the results of calculations for the system with coarsened mesh consisting of approximately 178 000 tetrahedrons. The ILU pre-conditioner is used in the calculations. Final residual of EM field calculation is $1.9 \cdot 10^{-10}$. The results (see Fig. 6) show that the preconditioner ILU works well also with the coarse mesh. The characteristic magnetic field and force density values are the same as in the case with the base mesh (the maximal difference is about 1%).



Fig. 6. Real part of the magnetic field in the system. Side view of the vertical cross-section (xz plane). Constant length vectors; magnetic field scale in T. System with coarsened mesh. ILU pre-conditioner, final residual $1.9 \cdot 10^{-10}$

2.4. The Dependence of the Obtained Results on the Value of Residual

In this subsection the solution dependence on the final residual value is studied using the system with refined mesh and ILU preconditioner. The following characteristic values of the physical fields in the atmosphere and melt domains are compared: B_{atm}^{max} , $B_{RE, melt}^{min}$, $B_{RE, melt}^{min}$, $B_{RE, melt}^{max}$, F_{melt}^{max} . Tab. 1 shows that the particular value of the residual in range $10^{-12}...10^{-8}$ practically does not affect the obtained solution, while for residuals in range $10^{-6}...10^{-5}$ convergence is not yet achieved.

Residual	$\mathbf{B}_{atm}^{max}, \mathbf{T}$	$B_{RE, melt}^{min}, \mu T$	$B_{RE, melt}^{max}, \mu T$	F_{melt}^{max} , N/m ³
$2.5 \cdot 10^{-5}$	0.01633140	19.6228	43.0640	0.00108830
$2.5 \cdot 10^{-6}$	0.00800944	19.6290	43.1103	0.00108876
$2.5 \cdot 10^{-7}$	0.00713624	19.5278	42.8081	0.00101320
$2.5 \cdot 10^{-8}$	0.00713650	19.6271	42.9169	0.000991315
$2.5 \cdot 10^{-9}$	0.00713653	19.6390	42.9296	0.000989748
$2.5 \cdot 10^{-10}$	0.00713653	19.6401	42.9308	0.000989613
$2.5 \cdot 10^{-11}$	0.00713653	19.6402	42.9309	0.000989596
$2.5 \cdot 10^{-12}$	0.00705442	19.6403	42.9309	0.000989595

Tab. 1. The dependence of the solution on final residual value.

Conclusions

The program *EM3D* has been used for calculations of the rotating magnetic field for 4" FZ system. Series of calculations have been carried out in order to study the sensitivity of the considered system to the density of the used mesh and various numerical parameters of calculations. The obtained results show that the ILU preconditioner gives correct results for all used mesh densities in the range from 170 000 to 600 000 elements while ILUT preconditioner underperforms for fine meshes (600 000 elements).

The characteristic values of magnetic field and force density distribution for the system with refined mesh are compared in several convergence states. It is shown that for residuals in the range from $2.5 \cdot 10^{-8}$ to $2.5 \cdot 10^{-12}$ the differences between characteristic values of physical fields are smaller than 1%.

Acknowledgement

The research was carried out with the financial support from ESF project at Latvia University with contract No.: 2009/0223/1DP/1.1.1.2.0/09/APIA/VIAA/008.

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