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Using of open source code library *OpenFOAM* for 3D magnetohydrodynamic calculations in semiconductor crystal growth technologies

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Abstract

To support the development of the industrial processes for CZ and FZ crystal growth, the system of mathematical models for the unsteady 3D modeling of liquid silicon laminar and turbulent motion under the influence of AC and DC electromagnetic fields is proposed. The corresponding codes on the basis of open source code object-oriented package *OpenFOAM* are developed. The structure of *OpenFOAM* package and its usage in creation of specialized solvers *FZsiFOAM* and *CZlesFOAM* is described.

1. Introduction

In order to grow the silicon (Si) single crystals industrially with all characteristics required for applications, basically, two methods are used: *Czochralski* (CZ) and *Floating Zone* (FZ). To support the development of the industrial processes for CZ and FZ crystal growth, the unsteady 3D modeling of liquid silicon laminar and turbulent motion under the influence of AC and DC electromagnetic fields must be carried out.

The usage of commercial solvers for FZ/CZ process modeling is encumbered with high license fees, which are especially high for the parallel calculations, and with problems to customize existing solvers. Another opportunity is to develop the computation code from the scratch, but as the practice shows, the implementation of computational codes for 3D fluid motion can be extremely complex, because the developers must implement not only the physical models and numerical methods but also auxiliary tools (pre-procesing/post-processing, parallelization on computer clusters etc.) in order to ensure an effective numerical simulation for large problems. Fortunately, the development efforts can be significantly reduced by using various open source code libraries which are very well developed nowadays. One of the most advanced open source code for the 3D fluid motion calcualations is *OpenFOAM* [1].

In present paper we propose the mathematical models and corresponding self developed codes *FzsiFOAM* and *CZlesFOAM* which are developed on the basis of open source code object-oriented package *OpenFOAM*. The codes *FzsiFOAM* and *CZlesFOAM* allow modeling of 3D liquid silicon laminar and turbulent motion under the influence of AC and DC electromagnetic fields during the CZ and FZ crystal growth processes. In present paper a brief structure of the object-oriented library package and general guidelines for the usage of the *OpenFOAM* functionality (e.g., classes) in creation of specialized solvers for the mathematical modeling of FZ and CZ crystal growth processes are given. By using our code in FZ process, 3D unsteady laminar fluid flow and corresponding transfer of dopants is

modeled. To simulate the CZ process numerically, the unsteady turbulent large eddy models (LES) are used for calculations of the 3D liquid silicon motion in the crucible. In both processes (FZ and CZ) the influence of electromagnetic fields is accounted by using a special *OpenFOAM* classes for the implementation of body forces in corresponding equations.

2. Open source OpenFOAM package

The *OpenFOAM* (Open Source Field Operation and Manipulation, [1]) package consists of a large set of C++ libraries which implement the necessary classes and objects for the creation of specialized applications. It should be noted, that besides the C++ libraries, the package contains also solvers for various standard problems and many auxiliary utilities. The solvers are designed to solve particular 3D problems in continuum mechanics, the utilities allow to perform a pre/post processing tasks like: mesh import or decomposition for parallel calculation runs or solution data export for visualization etc.

2.1. General Structure

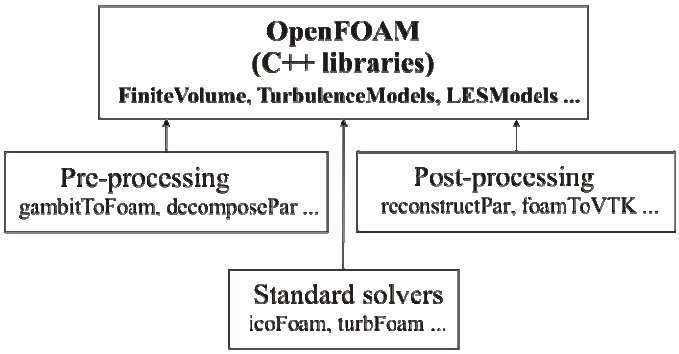

Fig. 1. The structure of *OpenFOAM* package

An overview of the structure of *OpenFOAM* package is shown in Fig. 1. The core part of *OpenFOAM* is implemented in C++ libraries with the aim to provide the support of various numerical methods (for example, finite volume method and finite element method), physical models (like, RANS turbulence models and large eddy simulation) and parallelization. Amongst various solvers for standard problems, the package contains, e.g., *icoFoam* solver for incompressible laminar 3D fluid motion. For the pre-processing, the package contains a comprehensive amount of utilities which can be used, for example, to import the 3D finite element mesh from such external packages as *Gambit* (utility *gambitToFoam*), *ANSYS* and other software. Additionally for the partition of 3D meshes, the special utility *decomposePar* is used, which is essential for parallel calculations on computer cluster. To visualize the calculation results the post-processing utilities (like, *foamToVTK*) are used to export the data to external 3D viewers (*Paraview*, *EnSight,* etc).

2.2. Essential Classes for the Creation of Specialized Process Solvers

To create the specialized solver on the basis of *OpenFOAM,* the mathematical problem, which describes the process, must be implemented in C++ by using the functionality of certain classes of the package (more details see in [2]).

First step is the discretization of the partial differential equations (PDE) and creation of the corresponding set of linear algebraic equations. The system of linear algebraic equations in *OpenFOAM* is represented by the following C++ classes: *fvMatrix* and *geometricField*, which implements the matrix of coefficients, vector of dependent variable and source vector (right hand side of the system) respectively. Each term of PDE can be represented in C++ by functions which implement the various differential operators, e.g., $\nabla, \Delta, \nabla\bullet$ and $\partial/\partial t$, and return the object of class *fvMatrix*. This approach maximise the similarity between the

mathematical formulation and corresponding C++ code, as shown below in example for the scalar diffusion equation with corresponding C++ code shown on the right side

$$\frac{\partial \phi}{\partial t} = \kappa \Delta \phi \quad \rightarrow \quad \text{fvm::ddt(phi)} == \text{kappa} * \text{fvm::laplacian(phi)}.$$

Second step is the definition of boundary conditions. Although for the basic types of boundary conditions (for instance, fixed-value or zero-gradient) there is available implementation in *OpenFOAM* package, some problems require the creation of specific boundary conditions. A new finite volume boundary condition can be implemented in C++ by creating the class which inherits from the class *fvPatchField* or other its descendants, like, *fixedGradientFvPatchField*, etc., and by adding the specific code for new boundary condition.

3. Specialized solvers for 3D hydrodynamic calculations during FZ/CZ processes

3.1. Description of the Mathematical Models

The unsteady 3D fluid motion during FZ/CZ processes are modelled by codes *FzsiFOAM* and *CZlesFOAM* for the cases with fixed phase boundaries. For the FZ process the calculations with 2D axially-symmetric model [3] and for CZ process the data from experiments, e.g., [4], are used to create the 3D representation of phase boundaries.

To model the 3D laminar fluid motion during the FZ process, the incompressible Newtonian fluid model with Bussinesq approximation for buoyancy forces is used with corresponding equations for the conservation of the momentum and for continuity:

$$\frac{\partial \vec{U}}{\partial t} + (\vec{U} \cdot \nabla)\vec{U} = 2\nabla \cdot (\nu \cdot S) - \nabla P + \vec{F}_B + \vec{F}_{EM}, \qquad \nabla \cdot \vec{U} = 0 \tag{3.1}$$

where $\vec{U}$ is velocity field; S is tensor of strain rate $S_{ij} = 1/2 \cdot \left(\partial U_i / \partial x_j + \partial U_j / \partial x_i\right)$; P is by density normalized pressure; $\vec{F}_B$ is buoyancy force $\vec{F}_B = -\alpha \cdot \vec{g}(T - T_{ref})$ with gravity vector $\vec{g}$, temperature T, global temperature reference T_{ref}, volumetric thermal expansion α, and kinematic viscosity ν; $\vec{F}_{EM}$ is electromagnetic force density created by electromagnetic (EM) AC or DC fields. The boundary conditions for the velocity field are as follows: 1) on the interfaces between solid silicon and melt, the fixed velocity field is set according to the angular rotation of crystal and feed rod; 2) on the free melt surface the shear stress is applied, which accounts the influence of the high frequency (HF) electromagnetic field and Marangoni forces. The temperature field is modeled by accounting the motion of the liquid silicon in the volume and heat flux on the free melt surface, which accounts the induced HF EM power and radiative heat losses according to law of Stephan-Boltzmann.

For the modeling of the 3D turbulent fluid motion during CZ process, the large eddy simulation (LES) model of Smagorinsky [5] is used. The Smagorinsky LES model is described also by the equation (3.1) with following changes. First, instead of molecular viscosity ν, the effective sub-grid turbulent kinematic viscosity ν_{ef} is used:

$$\nu_{ef} = \nu + (C_S \Delta)^2 \sqrt{2\overline{S}_{ij}\overline{S}_{ij}}, \tag{3.2}$$

where C_S is the empiric constant (usually in the range between 0.1 and 0.2); Δ is grid filter $\Delta = V^{1/3}$, where V is volume of the finite volume cell; $\overline{S}_{ij}$ is mean rate of strain. Second, the

rate of strain tensor S is replaced with mean rate of strain tensor $\overline{S}$. The boundary condition for the velocity field on the interfaces between crucible-melt and crystal-melt is set according to the rotation rate of the crystal and crucible respectively. On the free melt surface the slip type boundary condition is applied. Temperature field is calculated with the influence of the convection in the melt volume and with given heat flux density distribution along the free melt surface and interface between melt and crucible, known from the experiments or global thermal calculations.

The influence of EM field on the motion of liquid silicon in both models for FZ/CZ processes is determined by the term $\vec{F}_{EM}$ in (3.1), which in the case of AC fields is supplied from external EM field solver. To model the influence of DC fields, the corresponding EM force density depends on velocity field:

$$\vec{F}_{EM} = \sigma(-\nabla\varphi + \vec{U} \times \vec{B}) \times \vec{B}, \tag{3.3}$$

where σ is the electrical conductivity of the molten silicon; $\vec{B}$ is the magnetic field; φ is the electrostatic potential for witch the following coupled equation is solved:

$$\Delta\varphi = \vec{B}(\nabla \times \vec{U}) \tag{3.4}$$

with boundary condition $\partial\varphi / \partial n = (\vec{U} \times \vec{B}) \cdot \vec{n}$ where $\vec{n}$ is the normal vector at the boundary, and with one condition $\varphi(P) = 0$ to fix the value of the electric potential in one arbitrary point P in the considered domain.

3.2. Implementation in Computer Codes FZsiFOAM/CZlesFOAM

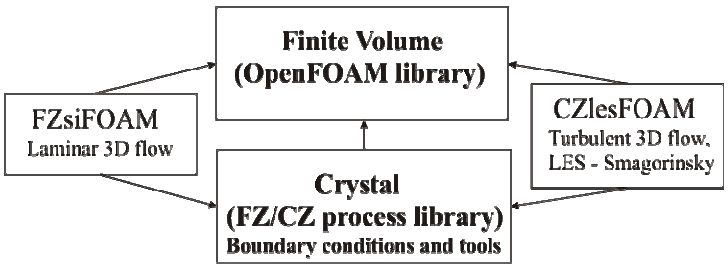

Fig. 2. The implementation architecture of codes *FZsiFOAM/CZlesFOAM*

The unsteady 3D fluid motion models for FZ/CZ processes were implemented in *OpenFOAM* based codes *FZsiFOAM/CZlesFOAM*. Since both solvers share a common classes, the corresponding source code were organized in three parts, where the first common part is library *Crystal* and other two parts are solver codes for the FZ/CZ process specific equation and iteration loop implementation. The library *Crystal* contains the classes for the implementation of boundary conditions as well as miscellaneous auxiliary tools (like, import of HF EM field, physical field probing, etc). In the implementation of all three parts, the *OpenFOAM* library *Finite Volume* was used. The mutual dependences of all mentioned components are shown in Fig. 2, where each arrow points to the used component.

4. Calculation Example

For the illustration purposes of the developed code, an example of calculation for the 6” inch FZ crystal growth system is shown below. The used finite element mesh has 180000 cells and is shown in Fig. 3. In Fig. 4 the calculated results by solver *FZsiFOAM* are presented together with the results of the special study for the influence of the parallelization on the

performance of the simulation. The used hardware was one cluster node with two quad-core Intel® Xeon® X5355 CPUs with 2.66GHz speed. More detailed information can be found in [6]. Another demonstration of the usage of code *FZsiFOAM* for the solar cell process modelling is given in [7].

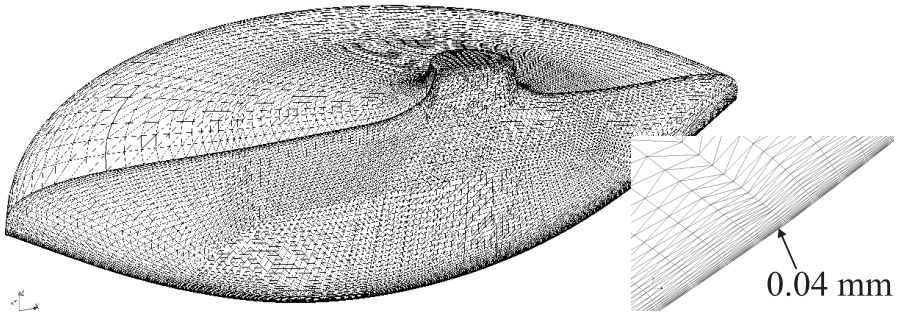

Fig. 3. Molten zone in the 6” FZ process, a half of the 3D hexahedral mesh used for calculations with solver *FZsiFOAM* and zoom-in of boundary layer at crystallization interface.

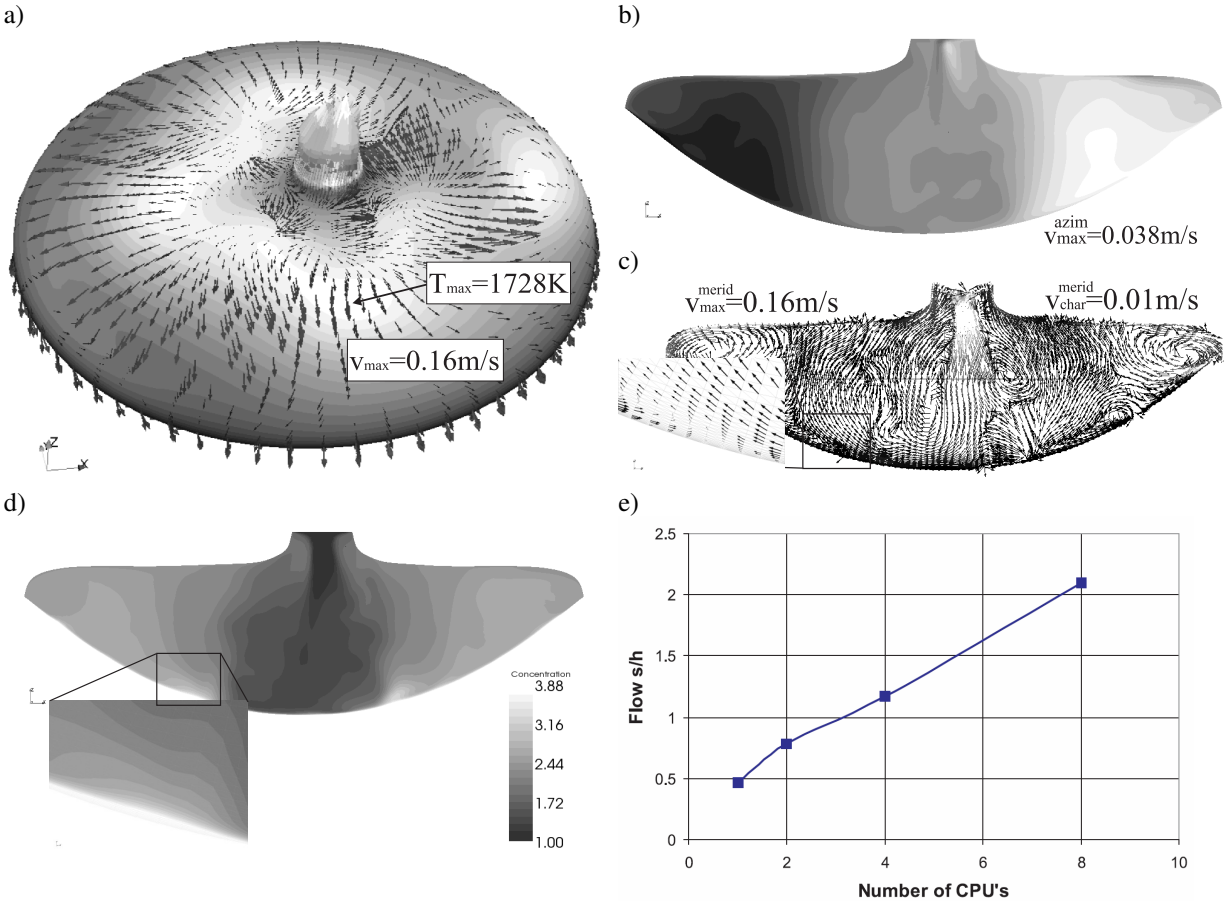

Fig. 4. Calculation results for 6” FZ crystal growth system and parallelization influence on the performance of the simulation: a) velocity vectors and temperature distribution on the free surface; b) azimuthal velocity in vertical cross-section; c) velocity vectors in vertical cross-section; d) concentration distribution and zoomed concentration boundary layer, e) physical time (in seconds) per computational time (in hours) as a function of the count of used processors.

Conclusions

The codes *FZsiFOAM/CZlesFOAM* for the modelling of unsteady 3D fluid motion under the influence of AC and DC electromagnetic fields during FZ and CZ crystal growth processes are developed. In the implementation of the codes the open source package *OpenFOAM* was used. Due to the previously implemented functionality in package *OpenFOAM*, the developed codes can be paralyzed easily on computer cluster and thus an effective simulation of large FZ/CZ problems can be carried out.

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