

CrystmoNet Remote Access Code for Czochralski Crystal Growth Modelling

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Abstract *CrystmoNet* code provides the ability of remote access by scheme *client-server* for the conjugated numerical solution of fluid and solid state mechanics problems in Czochralski crystal growth using a number of software modules: *Crystmo* and *Ansys[®]Fluent[®]* – for fluid mechanics, *MSC.Marc[®]Mentat[®]* – for radiative-conductive heat transfer and solid state mechanics, *Defects* – for defect formation and *Tecplot-360[®]* – as graphic postprocessor. Conjugated modelling is provided by the developed software interface. *CrystmoNet* code implements the *client-server* interaction at two operating platforms: *Microsoft[®]Windows client* receives the licensed remote access to *server*, where the above-mentioned software modules are installed for calculations at *Unix-like* operating system. The solution of conjugated fluid and solid state mechanics problems in Czochralski crystal growth is shown on the examples.

Keywords Modelling, Remote Access Code, Czochralski Crystal Growth

1. Introduction

Czochralski (Cz) crystal growth modelling has become an important scientific problem, which is the subject of many publications. On the one hand, this is due to the great practical importance of this technology and ever-increasing requirements to the crystal quality and size. On the other hand, there is the considerable scientific interest to a study of complex interaction of various physical processes influencing on the required crystal parameters.

Modern numerical modelling is focused on the conjugated solution of fluid and solid state mechanics problems in Cz crystal growth[1]. The basis of most these works is specialized software codes, which have their own grid generators, solvers and graphics tools.

An initial basis of the present work was a development of similar specialized code, too. It was based on our own numerical approach and software modules for conjugated heat transfer in Cz silicon (Si) hot zone[2-4] and the defect formation in dislocation-free Si crystals[5,6]. However, the development of such codes for new technologically important mechanical models of fluid and solid state usually faces with known difficulties caused by limited resources of research groups.

Therefore, in recent years we have developed *CrystmoNet*

program code on the basis of joint using our *Crystmo*, *Defects* modules and well-known commercial program codes for fluid and solid state mechanics problems: *Ansys[®]Fluent[®]* – for fluid mechanics (*Fluient* module), *MSC.Marc[®]Mentat[®]* – for radiative-conductive heat transfer and solid state mechanics (*Marc* and *Mentat* modules) and *Tecplot-360[®]* – for graphic representation of results (*Tecplot* module).

This paper describes the general approach for Cz modelling, the content of *CrystmoNet* and remote interaction of its modules and examples of Cz modelling. The examples are given in the application to Redmet-90M Cz puller for a large diameter Si single crystal growth[7]. The detailed discussions of the numerical results are contained in the published papers[8-11].

2. Description of Program Code

2.1. The General Approach for Cz Modelling

The conjugate radiative-conductive model (RCM) is applied to calculations of heat transfer in Cz hot zone (Figure 1). The approximation and solution of equations are carried out on the basis of finite element method (FEM). After FEM calculation the temperature distributions on the boundaries of melt and crystal are sent for calculations of convective heat transfer (CHT) in a melt by finite volume method (FVM). The calculated velocity field is used on next RCM iteration. The crystallization process and shape of liquid-solid interface (LSI) may be calculated in RCM or CHT models.

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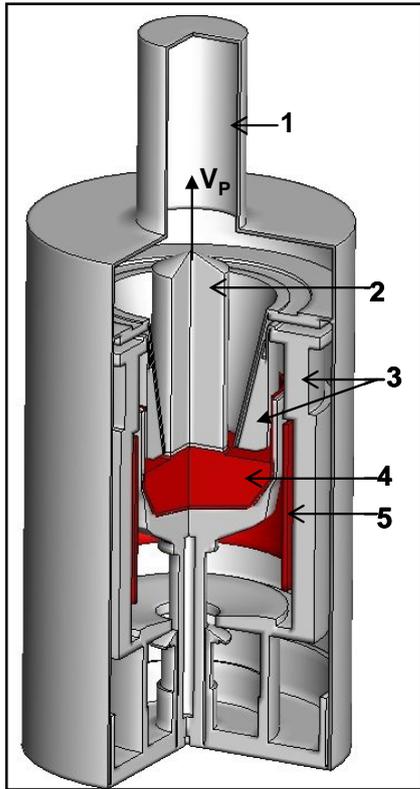


Figure 1. The hot zone of Redmet-90M Cz puller: 1 - tank, 2 - crystal, 3 - thermal shields, 4 - melt, 5 - heater; V_p - crystal pulling rate

2.2. The Composition of Program Code, the Remote User's Access and File's Exchange

CrystmoNet code provides the ability of user's telecommunication access by scheme *client-server* on two operating platforms: *MS Windows* - at user's computer and *Unix-like* - at the remote *server*. *CrystmoNet-Shell* module

and pre/postprocessor *Mentat* are installed on user's computer. *CrystmoNet-Shell* module is the shell program, which controls all operations of *CrystmoNet* code. The shell program manages a distributed computing environment and provides the interface between the system components, which are executed on *server* and *client* computer. *License* server and the subject-oriented - *Crystmo*, *Defects*, *Marc*, *Fluent* modules, and *Tecplot* - graphical postprocessor are installed at *server* computer. The data exchange between *client* and *server* is carried out according to the scheme shown in Figure 2.

The composition and structure of the code are designed for remote calculations with the use of high-performance servers. On a logical level the components of the code are distributed between the client's computer, *License* server computer and the computational *server* (computing cluster). *Client* computer with pre/postprocessor *Mentat* is used for data input: the geometry of hot zone and parameters, as well as for graphic output of contours and graphs on display and printer.

The modules - *Crystmo*, *Marc* and *Fluent* are executed on the *server* under *Unix-like* operating systems. The shell program - *CrystmoNet-Shell* opens the window with tabs on computer screen of user (see Figure 3: *Server.data*, *Marc+Crystmo*, etc.), which contains the input data for modules, the files to copy (from *client* to *server* and back), and command's buttons for a start of modules and *Tecplot* graphic postprocessor. The control of the number of the concurrent applications is managed by *License* server. The shell program executing on client's computer provides start/stop of code's components and data's transfer between them.

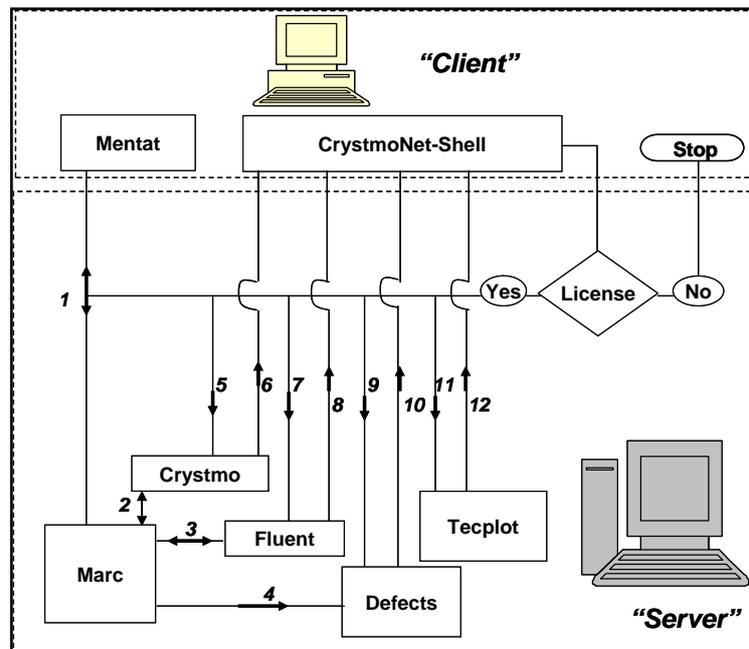


Figure 2. The functional diagram of *client-server* interaction with the directions of file exchange between modules for remote work with *CrystmoNet* code

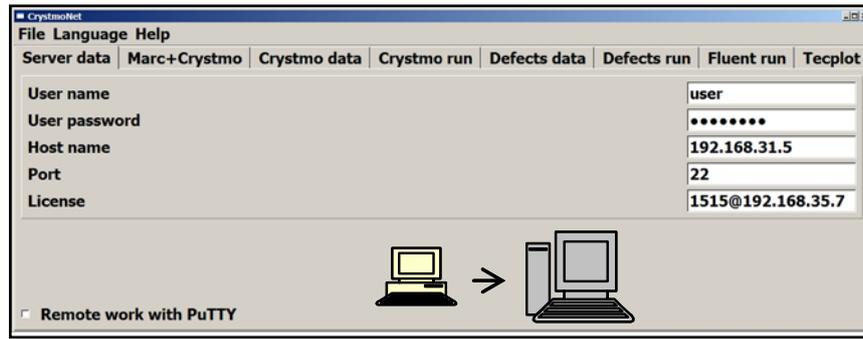


Figure 3. *Server.data* tab for user's registration for license work on the remote *server*

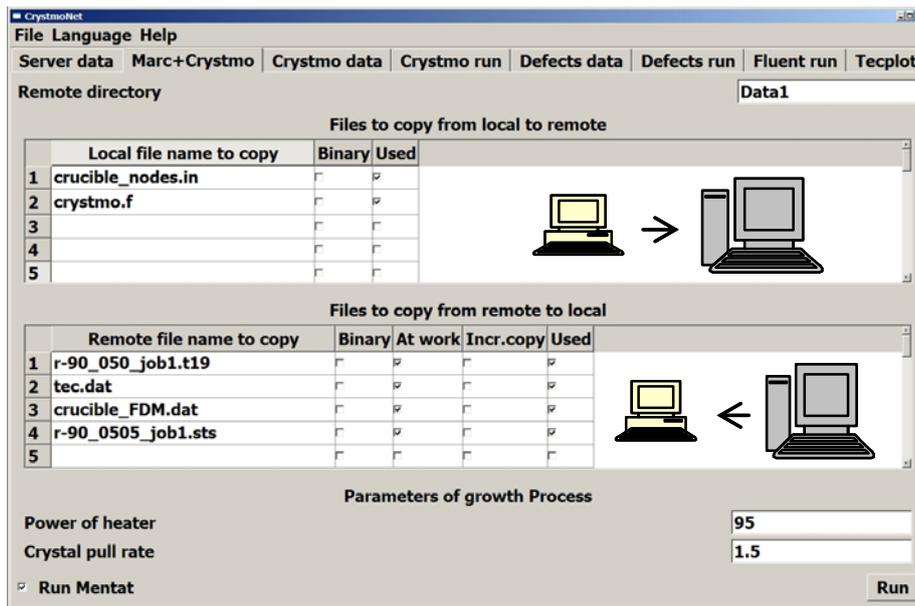


Figure 4. *Marc + Crystmo* tab for a transfer of files from *client* to *server* and back for executing the single module – *Marc* or *Marc+Crystmo* jointly executing

The work with the code begins by the run of the shell program on *client* computer and the license obtaining. With its help the remote mode is selected, and the location of code's individual components with the interaction between them is set. Besides, the shell program is used for the input calculated data of individual programs and for setting file's list for the data exchange between components running on different computers and for an execution of the modules themselves.

To obtain the license for remote work the following data are specified in *Server.data* tab (Figure 3): host name (or IP address), login name and password for user's authorization, and port of *ssh* communication.

The data of *License* server (host name or IP address and TCP communication port) are set in parameter - *License* in form $\langle port \rangle @ \langle host \rangle$. These data are provided by the system administrator.

The checkbox *Remote work with PuTTY* allows the display on user's screen of *server* terminal emulation for monitoring of the running processes.

Marc, *Fluent* and *Tecplot* modules have their own tabs for data input. For *Crystmo* and *Defects* modules in the shell program *CrystmoNet-Shell* the special *Crystmo.data* and

Defects.data tabs exist, which contain in tabular form the necessary input data.

Starting the calculation modules and the graphical postprocessor on *server* with the simultaneous *client-server* exchange of files begins with the *Run* button pressing in tabs of *Marc+Crystmo*, *Crystmo.run*, *Defects.run* and *Tecplot*.

An example of such a tab – *Marc+Crystmo* is shown in Figure 4, in which lists the files and their format for the send from *client* to *server* and back.

Directory on the *server* specified as *Remote directory* (for example, *Data1*) is used for the keeping the received and transmitted data of files during the running process. In the absence of such, it will be created by default during user's start.

Note that this tab provides two options for *Marc* module running. In the first case the calculation is carried out only by solver of *Marc* module and the checkbox on the button *Run Mentat* is missing.

In the second one for the conjugated calculation of *Marc* and *Crystmo* modules the checkbox on button - *Run Mentat* is on. For this option in the list of files copied to *server* the module *Crystmo.f* (Fortran's module) is included, which after clicking on *Run* button will be integrated into the object

environment of *Marc* with a creation the united *Marc+Crystmo* module for running.

For convenience of calculations in this box the following parameters are present: *Power of heater* and *Crystal pull rate*, which may be changed during *Marc* and *Marc+Crystmo* executing.

The conjugated calculation by *Marc* and *Fluent*, *Marc* and *Defects* modules is based on a file exchange between these modules.

The graphic representations by *Tecplot* module on *server* are executed on basis of the data in *Tecplot* format recorded as a result of the calculation modules and may then be copied as images on *client* computer.

2.3. *Marc* Module with *Mentat* Pre/postprocessor

Marc module includes *Mentat* graphic pre/postprocessor[12], in which the preparation of input data for *Marc* solver is carried out: the setting of the geometry of hot zone and its grid division into finite elements (Figure 5).

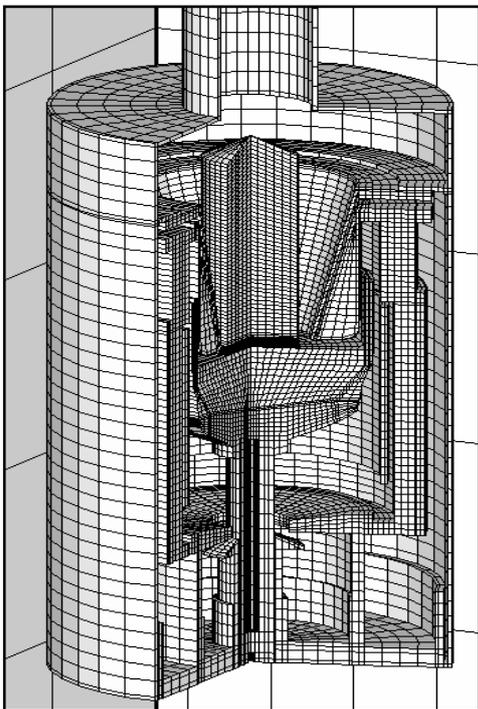


Figure 5. The illustration of FEM grid for Cz hot zone, which has been generated and plotted by *Mentat* module

The hot zone includes a number of components: the crystal, melt, heat shields, heater, tank (see Figure 1), each of which is specified by own material properties. The temperature on the outer tank wall is set. The crystal pulling rate and the heater power are setting by the values according to *Marc+Crystmo* tab (Figure 4).

The radiative heat transfer in Cz Si hot zone is considered in "gray-body" approach, and the view factors are calculated between the mutually visible surfaces. *Marc* solver is started in *Mentat* window with the corresponding parameters in "heat transfer" mode.

During the calculations *Mentat* postprocessor allows the

graphic output of results: one-dimensional graphs, thermal contours, isothermal surfaces and its animations.

The calculation of thermal stresses and strains in a crystal is carried out with taking into account of the calculated temperature field and by means of corresponding *Mentat* window with the inputting mechanical properties and by the run of *Marc* solver in "mechanical" mode.

One of the first applications of *Marc/Mentat* to Cz Si crystal growth has been carried out in [13], where the algorithm and its application to the conjugated radiative-conductive heat transfer in Cz hot zone has been described in details.

However, the convective heat transfer in a melt was not taken into account. Up to now an application of *Marc* module for Cz Si crystal growth is restrained by an absence of the internal program module for fluid dynamics modelling for the real thermal and Cz growth parameters corresponding to the large values of Reynolds, Rayleigh, Marangoni numbers.

2.4. *Crystmo* Module

Crystmo module calculates the hydrodynamics and heat transfer in a melt for Cz crystal growth. Three-dimensional Navier-Stokes and heat transfer equations are solved together in Boussinesq's approximation and cylindrical coordinates by FVM [2,3]. Physical parameters (density, viscosity, thermal conductivity and heat capacity) are assumed to be constant in a melt. The action of constant and rotating magnetic fields on the convective heat transfer in a melt may be taken into account [14]. The calculation grid, the adjusting and physical parameters are specified in tabular form in *Crystmo.data* tab.

The temperature distributions on boundaries of a melt are taking into account to the calculated data of *Marc* module for radiative-conductive heat transfer in Cz Si hot zone. For its transfer from FEM grid of *Marc* module on FVM grid of *Crystmo* module the data interpolation is done. The data for the file exchange between *Marc* and *Crystmo* modules are presenting in *Tecplot* format. For conjugated *Marc+Crystmo* execution the velocity components of a melt flow calculated by *Crystmo* are interpolated on FEM grid and then are passed to *Marc* in *Tecplot* format. File's exchange between *client* and *server*, and the starting of *Crystmo* module are done in *Crystmo.run* tab, which in appearance is similar to *Marc+Crystmo* tab (Figure 4).

2.5. *Fluent* Module

Fluent is used as the hydrodynamic module for Cz modelling, which has the additional possibilities: the solution of Navier-Stokes and heat transfer equations in a complex domain (for example, in a double crucible), with taking into account of crystallization and turbulent models of fluid dynamics. The physical parameters of liquid or solid materials (viscosity, thermal conductivity and heat capacity) may be temperature dependent. For preparation of input data for *Fluent* solver and for imaging the numerical results the

built-in image pre/postprocessor is used[15].

The examples of individual application of *Fluent* module for Cz modelling are known and fairly numerous, one of them is given in[16]. However, the examples of its joint using with *Marc* module are absent. In *CrystmoNet* code the conjugation of *Marc* and *Fluent* modules is built on basis of file's exchange. For this purpose, we have elaborated the special C++ subroutines, which allow user's input/output of data: the input of the temperature distributions on boundaries (of melt and crystal) in according with *Marc* results and output of velocity components in a melt after *Fluent* calculation. During the data transfer the same interpolation as for conjugated *Marc+Crystmo* calculations is done.

2.6. Defects Module

Defects module calculates the recombination and diffusion of intrinsic point defects - IPD (vacancies and Si interstitials)[5] and the microdefect's formation[17] in growing dislocation-free Si single crystals. For this calculation the crystal temperature field is used, which has been calculated by *Marc+Crystmo* or *Marc+Fluent* modules.

The system of equations for calculation of IPD concentration and the microdefect density is solved by finite difference method (FDM) in the crystal. FDM grid and the physical parameters are set in tabular form in *Defects.data* tab. The file exchange between *client* and *server*, and the run of *Defects* module is done in *Defects.run* window, which in appearance is similar to *Marc+Crystmo* tab (see Figure 4). The data for file exchange between *Marc* and *Defects* modules are set in *Tecplot* format. During file exchange the data interpolation is done as in conjugated calculation by *Marc* and *Crystmo* or *Fluent* modules.

2.7. Tecplot Module

Tecplot module is used as the universal and most efficient graphic postprocessor that does the graphic images of numerical results obtained by different numerical methods (FEM, FVM and FDM). The graphic tabs of *Tecplot* module is simple and easy for graphic editing of numerical results[18]. The run of this module is done in *Tecplot* window (Figure 4).

The file exchange between *client* and *server* provides loading the numerical results in *Tecplot* format for each of the calculation modules (*Marc*, *Crystmo*, *Fluent* and *Defects*). An analysis of the numerical solutions is done by graphic tools of *Tecplot* module and by means of *Mentat* and *Fluent* postprocessors, too.

3. Examples of Cz Modelling

Let's consider the examples of the application of *CrystmoNet* code for the conjugated Cz modelling. For adequate modelling of thermal field in a crystal it is important to take into account of the melt convection and the crystallization process. The convective heat transfer in a melt

is considered in the crucibles of different shape (usual single crucible, double or more complex crucibles) under the effect of crystal or/and crucible rotation, thermal gravitational and thermal capillary convections. For the semiconductor melt (such as Si) may be taken into account the constant and rotating magnetic fields. The calculations of Cz heat transfer are based on the conjugation of RCM model of *Marc* module and CHT models of convection in *Crystmo* and *Fluent* modules. The calculations of stress state and microdefect formation in a crystal are done on basis of the results of such conjugated thermal modelling in *Marc* module (for "thermal mechanical" tasks) and in *Defects* one respectively.

3.1. Conjugated Heat Transfer

For *Marc+Crystmo* conjugated option the calculations are carried out in the following sequence. At the beginning the calculations are carried out by *Marc* module for conductive-radiative heat transfer (without taking into account of velocities field in crystal and melt) and at an initial power of heater. For taking into account of the crystallization in *Marc* module the transition layer between melt and crystal in the temperature range $T_S < T < T_L$ ($T_S = 1678$ K – solidus, $T_L = 1688$ K – liquidus) is setting, in which a latent heat of crystallization is released. The temperature field in Cz hot zone is calculated with iterative correction of heating power till the value, corresponding to the desired position of LSI edge of on the lateral crystal surface (see the control point 6 in Figure 6). According to the results of this calculation in file exchange for *Crystmo* module the following data are recorded on the melt geometry: LSI shape taken as the melting temperature contour $T_M = 1683$ K for Si, fixed shapes of free melt surface and crucible and the temperature distributions on these boundaries (bottom and lateral crucible walls, the free melt surface as shown in Figure 6).

Further with taking into account of this file *Crystmo* module is started and it calculates the heat transfer and the velocities field in a melt without crystallization. This velocities field is written to the file exchange for a copy into *Marc* module for the next iteration of conjugated calculation. For the next iteration the calculations by *Marc* module are executing with taking into account of the velocities field in a melt, the crystal pulling rate and crystallization. It may change the previous shape and location of LSI, therefore an iterative adjustment of heating power is done till the value corresponding to the desired position of the control point 6 in Figure 6. *Marc+Crystmo* iterations are continued till the stabilization of heating power and position of the control point.

In general, the conjugated *Marc+Fluent* calculations are repeating *Marc+Crystmo* sequence of run. The difference is concluded in taking into account of the crystallization, which is done in *Fluent* module. In this case *Marc* module is used only the calculations of the radiative-conductive heat transfer in Cz hot zone. The temperature distributions on the boundaries of melt and lateral crystal surface (1-4 in Figure

6), which taken from *Marc* calculation are passed into *Fluent* module. *Fluent* module calculates the heat transfer jointly for the crystal and the melt with taking into account of the crystallization and crystal pulling rate. The melt geometry is passed from *Fluent* module in *Marc* module with the calculated LSI shape and velocity field in melt and crystal.

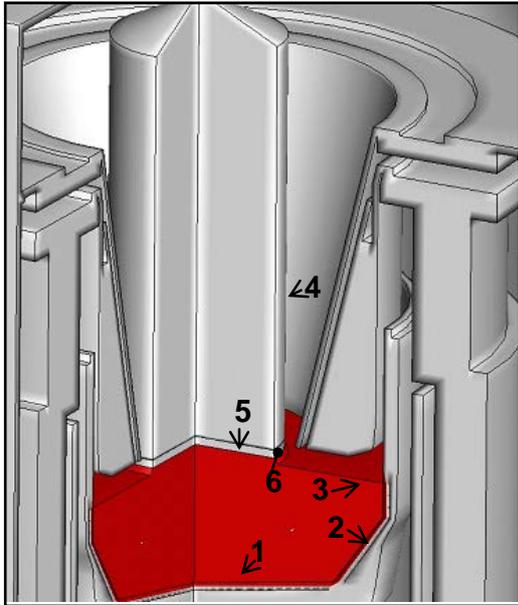


Figure 6. The marked boundaries of a melt, on which the temperature distributions are recorded in the exchange file by *Marc* module for the following using in *Crystmo* or *Fluent* modules. Here: 1, 2 – bottom and lateral crucible walls, 3 – free melt surface, 4 – lateral crystal surface, 5 – layer of crystallization, 6 – control point on LSI edge

The heating power and crystal pulling rate are adjusted in *Marc+Crystmo* tab without checkbox on *Run Mentat* button that corresponds only *Marc* module run (see 2.2). The power corresponding to crystal overheating may cause the considerable upwards displacement of LSI relatively to the control point of meniscus (Figure 7a).

As a result, the required position of the control point may be reached by the iterative correction of heater power and corresponding recalculation of hydrodynamics by *Fluent* module. This result is shown in Figure 7b, and it corresponds to the concave LSI shape. The corresponding distribution of temperature contours in the hot zone of Redmet-90M puller is shown in Figure 8.

The above calculations correspond to a single stage of crystal growth for the fixed geometry (the crystal length, the melt depth and the crucible position).

Quite a number of such stages are considered for the complete thermal analysis of crystal growth (for different lengths of growing crystal) at the conjugated calculations of dynamics of defect formation and stress fields in a crystal. The results of these calculations are collected in a database. The time-interpolation for adjacent stages is used for smooth changing in the temperature field. On this basis, the complete thermal history of growth process may be presented, which shows the time-development of thermal field in hot zone and growing crystal.

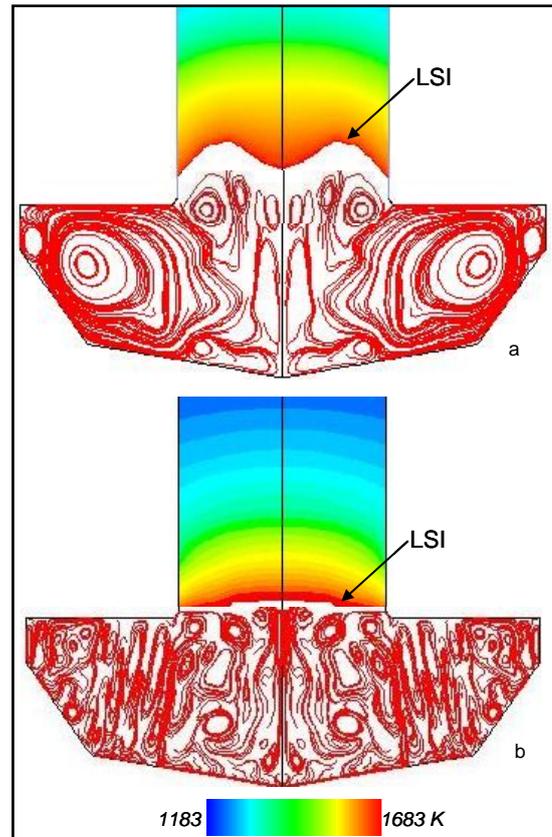


Figure 7. The thermal field in crystal and streamlines in melt after conjugated *Marc* and *Fluent* calculations: a – W-shape of LSI for large heater power, b – concave shape of LSI for optimal heater power

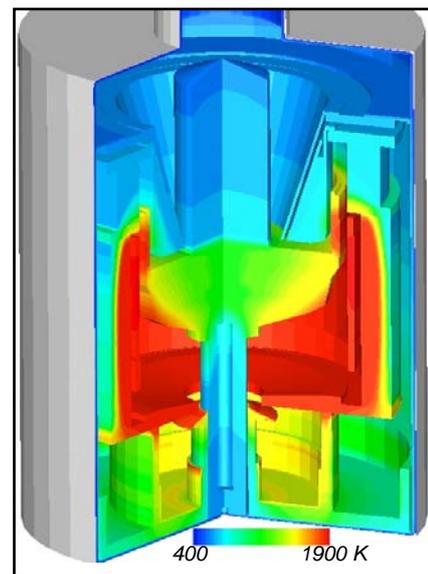


Figure 8. The thermal field in Cz hot zone after conjugated *Marc* and *Fluent* calculations

3.2. Conjugated Stress and Defects Calculations

During crystal growth process the thermal conditions have a significant influence on the stress state in the large diameter Si single crystals. By means of *Marc* module it was calculated the thermal stress state of a 100 mm diameter Si single crystal on one growth stage for an estimation of the

appearance of critical stresses, which cause the plastic deformation and the generation of dislocations (Figure 9a). The calculated values do not exceed the critical stress. Its maximum value (7.6 MPa) is achieved on the lateral crystal surface closely to LSI and it is caused by the largest temperature gradients in this area. The stress decreases rapidly with the increasing distance from LSI.

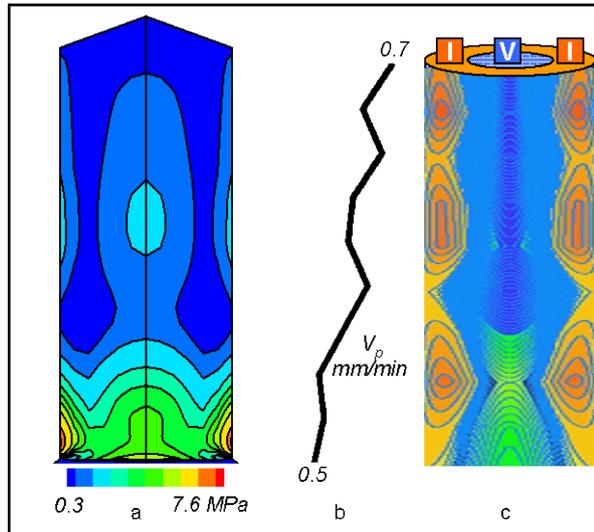


Figure 9. The conjugated modelling the stress state and defect formation in Si growing crystal: a – the field of von Mises stress; b,c – the change of pulling rate V_p during growth process and corresponding I/V-distributions of microdefects

The thermal conditions have the significant influence on the recombination of intrinsic point defects and the formation of microdefects in dislocation-free Si single crystals. By means of *Defects* module the distribution of microdefects in a 150 mm diameter Si single crystal was calculated with using the data of its thermal growth history and taking into account of changing the crystal pulling rate (Figure 9b,c). The image of microdefect distribution in the crystal is following: Si interstitial species (I) are concentrated closely to lateral crystal surface, but the vacancies (V) are located in the crystal center. The changing shape of I/V boundary corresponds to the changing crystal pulling rate.

4. Conclusions

Until now for Cz crystal growth modelling there is the limited use of well-known commercial codes of extensive application: the such as *Ansys®Fluent®* – for fluid mechanics and *MSC.Marc®Mentat®* – for solid mechanics problems. Its usual application is related with a single solution of non-conjugated problems. It may be the radiative-conductive heat transfer, melt fluid dynamics or stress state in a crystal.

For the conjugate Cz modelling the problem-oriented Cz commercial codes are used widely (*CGSim®*, *FEMAG®*, *STHAMAS®*, *CrysMAS®* et al).

For many years these codes were developing in close

contact with Cz technological practice and therefore well adapted for such calculations. It is an indubitable competitive advantage of these codes. The disadvantage is a rather narrow set of physical models, especially for solid mechanics in comparison with *MSC.Marc®Mentat®*. Moreover the user is limited by possibilities of models included in these codes, and the independent integration of user's or other program modules is impossible without the developers of these codes.

The present paper reviews one possible approach of integrated use of user's (author's) *Crystmo* and *Defects* modules and the codes of extensive application in Cz modelling: *Ansys®Fluent®*, *MSC.Marc®Mentat®*, *Tecplot-360®*.

This approach is implemented in *CrystmoNet* code and allows the remote access by means of *client-server* scheme. We took into account the desire of the majority of our colleagues and especially students for a work on their own computers (*client*) with using the most widely operating systems (*MS Windows*).

It was elaborated non-standard network version of *CrystmoNet* code for a work at two operating systems: *MS Windows* – for user's work on *client-computer* and *Unix-like* – for all calculations on a remote *server*.

The program-shell of *CrystmoNet* code manages by the distributed computing environment and provides the interface between the code's modules, which function on *server* and *client* computers.

This version may be easily expanded by user's own modules for special applications of fluid and solid state mechanical problems emerging in Cz crystal growth technology.

In the above examples of Cz modelling for conjugated heat transfer, stress state and defect formation in a crystal there is presented a little part of parametric calculations carried out by *CrystmoNet* code during an elaboration of hot zone for Redmet-90M Cz puller.

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