Design of control system for growing crystals with desired properties

Mark M. Gonik, Victor I. Boevkin, Anastasia V. Lomokhova, Michael A. Gonik

INTRODUCTION

In order to grow high quality crystals, one needs to find optimal thermal conditions of crystallization and to realize them during the entire run of the technological process. Solution of this problem is obtained by using a control system of a temperature distribution in the growth furnace, which enables to realize the required crystallization regime with a high accuracy. Recently, a strategy of the choice of optimal thermal conditions of crystallization is based on numerical investigations of heat and mass transfer processes in the growth set-up. The numerical model is also necessary for development of a control system, since it enables to thoroughly investigate the furnace as a control plant and to carry out an accurate design of control algorithms. Basing on a complex of the technology and required mathematical software of numerical calculations, it is possible to set the problem of development the control system directly of growing crystal quality. That is by such properties which determine its perfection: the structure homogeneity, the distribution of dislocations and other growth defects. For conventional methods of crystal growth, such as Czochralski and Bridgman ones, it is extremely difficult to build a precise and effective model because of the intensive and unstable character of convection in the melt. In the AHP technique (Advances Heating Method) [41], convection in the melt closed to the growing crystal is negligible [52], so it allows us to build a model for solving both direct and inverse problems with high precision and with low computing costs. In the paper the authors present a first attempt to develop a software and hardware complex for the realization of the growing crystal quality control by the AHP method.

I. AHP CRYSTAL GROWTH METHOD

In the AHP method (see Fig. 1), the additional heater is located close to the phase interface and divides all the volume into two zones Z1 (between the AHP heater and the crystal) and Z2 (for melt "preparation" above the AHP heater) drastically changing the character of flow close to the growing crystal. During crystal growth, the crucible is pulling downward, while AHP heater is held in position. As a result, forced melt flow from zone Z1 into Z2 occurs. The melt flow in zone Z1 becomes weak, laminar and practically stationary one.

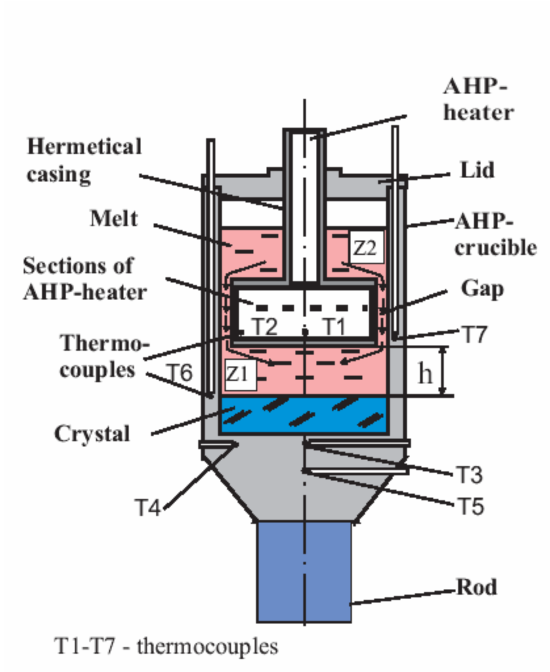

Figure 1: AHP crystal growth set-up.

II. PROBLEM OF THERMAL FIELD CONTROL.

Thermal field in the crystallization zone is formed by four controlled sections of the background heater and by one (or two) sections of the AHP heater. The temperatures are measured by thermocouples placed in the crucible and AHP heater. The basic control points characteristic to describe the temperature field are located over all boundaries of the melt-crystal area: T1 is in the center of the AHP heater, T2 - at its periphery, T3 is in the bottom of the crucible and T7 - in the crucible wall near the background heater and close to the solid-melt interface.

The most important stage of the technological process is pooling of crucible together with growing crystal and cooling, which determines the quality of the crystal. As governing for the control system, points T1 and T3 (Fig. 2) are chosen. In accordance of AHP growth regime, temperature T1 is to be kept constant, while temperature T3 should be changed with time due to given law (linear as a rule). The requirements of the maintenance accuracy of input temperatures for the developed control system are 0.05 – 0.1K, which allow to prevent the crystal growth rate instability and, as a result, the capture of impurities.

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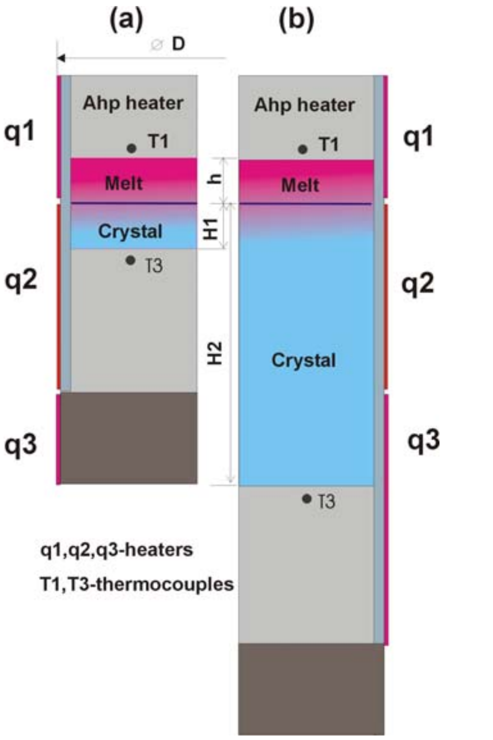

Figure 2 Calculation area for initial (a) and final (b) stage of crystallization: H1=10 and H2=45 mm are heights of a crystal , h=10 мм is the height of a melt, D=60 mm – the diameter of a crystal; q1,q2,q3 – fluxes of the heater sections.

The features of the object to be studied are that (i) it changes its own inertial properties as a result of redistribution of materials during the crystallization process; (ii) the crucible together with a crystal and melt changes its location relative to the controlling heaters; (iii) the process of growth is essentially connected with the nonlinear process of extracting/absorption of a latent heat during melting and crystallization of the material. So the control object should be considered as a nonlinear and unsteady one.

Solution of the stated problem is achieved by designing and applying algorithms of adaptive control for considering MIMO plant.

III. CONTROL OF GROWING CRYSTAL PROPERTIES

The problem of temperature field control is a component part of the growing crystal quality control. A scheme of developing control system of crystal properties is shown in Fig. 3. The factor describing such crystal properties as thermal stresses in crystal, density and distribution of dislocations is a complex quality factor **Q.** Mentioned properties are determined by a shape of the solid-melt interface and a temperature gradient in the crystal, which are affected in its turn by the thermal field created in the furnace. In the system under review, a numerical model (*Direct Model*) calculates quality factor **Q** on the basis of temperature distribution **T** measured by thermocouples over the boundary of the melt-crystal system. During crystal growth, current changes of the quality factor **Q** is tracked by a feedback and with help of *Inverse Model*; due to solving the inverse problem, the optimal temperature distribution **T** is determined. In that way, a control loop of the quality factor is realized. The internal loop of thermal field **T** control includes algorithms of the plant identification in the closed loop and control parameters *Adaptation*. The temperature loop could use the numerical *Predict Model* for Model Based Control technique.

IV. INSTRUMENTATION

To present day, we use for simulation the already developed software such as KARMA [3], Cats2D [4] as well as CGSim [5]. By means of them it has been reached considerable advance of comprehension of processes taking place during growth by AHP method [6,7,8,9]. But they do not meet necessary requirements for this problem. Therefore we have developed own software FEAP (see Fig. 4), which allows modeling the thermal process in the melt-crystal system in real time of the growth process [9].

The developed instrument enables to make identification of the control object in relation of temperatures **T**, to investigate its features referred above and to modify its parameters. The model permits to study process in every point of the melt-crystal system, both inside the crucible and round its bottom. Additionally, we have realized possibility of control algorithm testing directly with a numerical model.

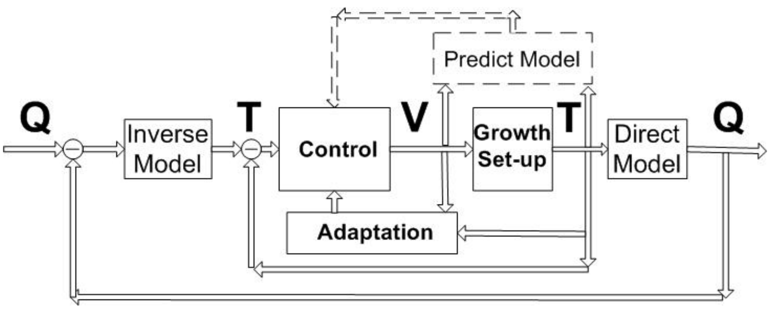

Figure 3: Algorithm of control system for crystal growth.

It enables to estimate the algorithm effectiveness most fairly. The test complex carried out has shown a fine coincidence of calculations and experimental results.

V. RESULTS

Investigation of the plant with help of the developed model has been carried out. Results of identification of two-dimensional MIMO plant described by equation (1) with transfer functions have been obtained. Temperatures T1 and T3 are controlled variables, fluxes q1 and q2 are manipulate ones. G11(s), G23(s), G13(s), G21(s) are corresponded component of matrix transfer function **G:**

$$\begin{bmatrix} T1(s) \\ T3(s) \end{bmatrix} = \begin{bmatrix} G11(s) & G21(s) \\ G13(s) & G23(s) \end{bmatrix} \times \begin{bmatrix} q1(s) \\ q2(s) \end{bmatrix} \quad (1)$$

The transfer function matrix for the initial stage (see fig. 5a) $\mathbf{G_A}(s)$ and the final stage (see fig. 5b) $\mathbf{G_B}(s)$ have been presented by equation (2) and (3).

$$\mathbf{G_A}(s) = \begin{bmatrix} \frac{0.00301}{(4s+1)(155s+1)} & \frac{0.00351}{(18s+1)(167s+1)} \\ \frac{0.00563}{(18s+1)(168s+1)} & \frac{0.0086}{(7s+1)(167s+1)} \end{bmatrix} \quad (2)$$

$$\mathbf{G_B}(s) = \begin{bmatrix} \frac{0.00295}{(4s+1)(180s+1)} & \frac{0.0037}{(10s+1)(221s+1)} \\ \frac{0.00268}{(83s+1)(207s+1)} & \frac{0.0052}{(32s+1)(226s+1)} \end{bmatrix} \quad (3)$$

Moreover, we have revealed an important feature of this object. Cooling (crystallization) and heating (melting) curves in points located close to the crystallization front have a great hysteresis (see fig. 4) in contrast to points located far away from the crystallization zone.

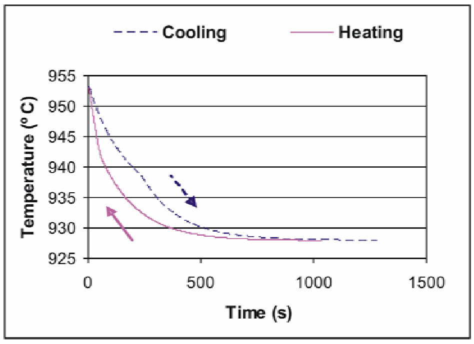

Figure 4: Temperature transient curves in the open loop for point far away from (a) and close to (b) crystallization front (T=937 ºC).

VI. CONCLUSIONS

Authors in cooperation with other teams are carrying out a complex of work for realization of the task of thermal field control and parameters of growing crystal quality control. The results of development and application of control algorithm for existing non- stationary and nonlinear MIMO plant instead of PID regulators applied to date are presented. The influence of crystal growth velocity variation on control precision is considered.

A high-accuracy control system being under development will make it possible to improve quality of crystal being grown by AHP technique and to exceed achievements of conventional growth methods.

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