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► To cite this version:

J. Glownia, H. Polcik. Numerical optimization of the solidification conditions of monocrystals of the Fe-Cr-Ni alloys. Journal de Physique IV Proceedings, 1993, 03 (C7), pp.C7-1217-C7-1222. 10.1051/jp4:19937187 . jpa-00251819

HAL Id: jpa-00251819

<https://hal.science/jpa-00251819>

Submitted on 1 Jan 1993

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Numerical optimization of the solidification conditions of monocrystals of the Fe-Cr-Ni alloys

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Abstract

In the recent investigations of foundry processes, numerical experiments apart from physical ones are the basic tools. In the works carried out up till now and concerning solidification and cooling processes of castings, numerical methods have been mainly applied to describe temperature distribution during the time of the processes.

In the author's own investigations, methods of control theory are used to determine the assumed and experimentally tested temperature distribution in the directional solidification of Fe-Cr18-Ni single crystals. The optimum solidification conditions (gradient of the temperature, rate of crystalization) were obtain by means of simulation.

The main purpose of this simulation problem was point out, that algorithm allow to obtain assumed temperature in the liquid phase, by the control of the heat flow in the solid region.

1. Introduction

In the most heat flow models treat the solidification process rather simply, e.g. by a temperature distribution during the time of the freezing. More complicated solidification model accounting for the control of crystallization conditions by the freezing rate or microsegregation effects of several alloying elements are used rather seldom [4,10,11]. Sometimes the continuity equations are solved separately for the solid and liquid phases, with appropriate boundary conditions being imposed at the moving solid-liquid interface. In the first stages of the modeling of solidification heat transfer, an application of a finite difference method (FDM) to castings was limited by the thermophysical properties of the mould and alloy.

Since the 1980s, there has been a significant growth in the number of programs and modeling techniques [2,5]. One of such system (The Michigan Solidification Simulator-MSS) determines problems of energy transfer (steady-state) with nonlinear material properties, phase change and bulk-flow velocity. The validation of the program has been performed, first for one-, or three-dimensional transient heat transfer without solidification, second-for a case involving a latent heat term but zero superheat, and finally, for a variety of axisymmetric and three-dimensional examples involving the solidification of metals, where validation was undertaken experimentally from thermocouple measurements. Very good agreement was obtained between simulation and experiment for gray iron casting, Al-Si casting and carbon steel railwheel [6].

All these finite-element methods (FEM) are used for different casting configurations, in which isotherms are shown in the cross-sections of the casting. Such isotherms (liquid metal) from that simulation indicate, that the casting should be sound due to the directional solidification (no shrinkage defects).

The main task of our research is elaboration a such way of cooling control during directional solidification, in which the assumed temperature as well as temperature gradient can be achieve. So that, assumed temperature distribution in the chosen thermal casting points will be our main task. In the rest thermal points of casting, the temperature distribution can be obtain by interpolation.

2. Materials and experimental procedure

The single crystal casting process is shown schematically in Fig.1.

In each case, the alloys were available as a rod with a machined outer surface and 8 mm diameter. The rod (specimen) was inside a ceramic mold (pure alumina) seated on a water cooled chill. Grains are nucleated on the solid-liquid (S-L) interface near the bottom of the chill and grow parallel to the unidirectional temperature gradient. Whole process was controlled by the temperature gradient at S-L interface and the rate of solidification (withdrawal the chill with mould from the hot zone of the furnace). Four PtRh18 thermocouples with 0.1 mm dia. were placed in the centre of the specimen. The ends of thermocouples were transferred 5 mm each others. In this case, when the lowest thermocouple indicated the

Fig.1. Schematic drawing of directional solidification process.

temperature of the S-L interface, the next two could controlled the distribution of the temperature ahead of the interface. The fourth thermocouple was in a solidified matrix and could measure the heat flow during the freezing of the alloy (Fe-Cr18-Ni9%).

3. Numerical procedure for control of directional solidification process

Let us take, that the solidification model can be written in the form :

$$\frac{\partial T}{\partial \tau} = a \frac{\partial^2 T}{\partial s^2} \quad (1)$$

$$a = \lambda / \rho c$$

λ - thermal conductivity

c - specific heat

ρ - specific mass

According to the practical experience we can assume, that λ is the same and equal for the whole solidification region (liquid state, solid-liquid area and solidified matrix). In the equation (1) it is needed to take into account crystallization heat, it means we have to improve the temperature on the way : liquid, mushy zone and solidified part. The formula for temperature improvement can

be found in the work [9]. Without detail consideration model (1) can be written in the normalized form as :

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} \quad (2)$$

Assuming for the variable x the discretization step h , equation (2) can be transferred to the form :

$$\begin{bmatrix} \dot{v} \\ \vdots \\ \dot{v} \end{bmatrix} = \frac{1}{h^2} \begin{bmatrix} -2, & 1, & 0, & \dots, & 0 \\ 1, & -2, & 1, & \dots, & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0, & 0, & 0, & 1, & -2 \end{bmatrix} + \frac{1}{h^2} \begin{bmatrix} \dot{v}_0 \\ \vdots \\ \dot{v}_{M+1} \end{bmatrix} \quad (3)$$

We shall treat the function $V_n(t)$ as an approximation of the values $V(x,t)$ in the points of the space $x = n h$ (Fig.1, $M=4$), where :

$$n = 1, 2, \dots, M; \quad h = 1/(M+1).$$

To system (3) which is now in the form :

$$\dot{V} = A V + B U \quad (4)$$

where :

A, B - matrices, U - controls (in our case U means temperature);

can be applied some control theory methods.

For systems (4) some numerical algorithms and computer programs were elaborated. These programs may be used to calculate optimal control, which transfers system (4) from its initial point V_0 to the origin $V_k = 0$:

a. - in the minimum time;

b. - in the given time (and minimum energy consumption).

In the case :

a. controls are in the bang-bang form : $-1, +1, -1, +1, \dots$

b. controls are : $-1, 0, +1, 0, -1, 0, \dots$

The main tasks of the above mentioned programs is time switching calculation.

If we consider the directional solidification problem, it means we have the only one control. Our task will be finding the times switching for the change the temperature of cooling medium. The values of the temperature of switching medium are depended on the initial temperature of liquid metal and the target point (temperature), we are going to achieve. As a result of utilization the above described methodology, to achieve the target point in the shortest time (case-a.), we obtain the times switching : $t_1, t_2, t_3, \dots$, in which we have to change the temperature of cooling medium.

For instance if the initial temperature is equal 1500°C and we want to achieve 1100°C as a result of control, the values of temperature of cooling medium will be :

$$0 \div t_1 : 800^\circ\text{C}; \quad t_1 \div t_2 : 1500^\circ\text{C}; \quad t_2 \div t_3 : 800^\circ\text{C}; \dots$$

Of course, after first time switching t_1 , we can calculate the new series of time switching again and assume the new cooling medium temperature, for instance : $1300^\circ\text{C}, 900^\circ\text{C}$.

different temperature gradients (Fig.3). These results point out that the method of the control of the temperature gradients will be useful for numerical simulation. The other problem is control of heat flow in the matrix. This technique is elaborated now and will be discuss in the next papers.

Fig.3. Temperature distribution of the sample during the solidification process.

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