

Numerical and Experimental Evaluation of Stray Grain Formation During Single Crystal Casting

M. Ghanbari^{1*} S.G. Shabestrai²
M.R. Aboutalebi³

1- Introduction

Single crystal blades are an important component in high power gas turbine engines. The production of single crystal blades improves high temperature rupture and creep resistance. This improvement is due to the elimination of high-angle grain boundaries and the formation of <001> crystal orientation. To produce a single crystal during directional solidification, a unidirectional thermal gradient is formed in the solid/liquid interface and then the interface is moved at a constant rate. Preferentially oriented grains are established in competitive growth. In materials with a cubic crystal structure, the <001> direction is known as the preferred crystal orientation.

To produce the single crystal structure, a directional solidification front should move in a thermal gradient. Therefore, grains with preferred <001> direction remain in the competitive growth mechanism. In the first stage, a preferred texture is produced during directional solidification and then a single grain is selected using a crystal selector. One of the most usual defects in the single crystal growth is stray grain formation which causes mechanical degradation in superalloys. The as-solidified structure of the cast alloys is a function of thermal gradient and growth rate during directional solidification. These parameters are affected by the furnace temperature, the moving speed of the sample during directional solidification process and the cooling rate of the sample. Columnar to equiaxed transition (CET) occurs as a result of the alloying system, casting size, heat transfer coefficient and nucleation conditions. Hunt developed a model to describe the conditions associated with the CET phenomena. Also, Wang and Beckerman developed a model to predict the position of the stray grain in the sample. According to Hunt's criterion new grains in the solidification front form in the

undercooled zone. Hunt's criterion is described as Equation 1.

$$f_g = n_g \frac{4\pi}{81} \frac{A^3}{(GR)^3} \left(\left(\frac{R}{A} \right)^2 - \Delta T_n^3 \right)^3 \quad (1)$$

According to this equation, the formation of equiaxed grains depends on the thermal gradient in the melt and the growth rate of the solidification front. So, to prevent the formation of equiaxed grains, thermal gradient and growth rate should be controlled.

2- Experimental

The goal of this study is to predict the conditions of the stray grain formation using cellular automaton finite element (CAFE) method. Procast simulation software and CAFE module were used in this study. The following energy equation is used in this software to predict the temperature in the domain:

$$\rho \frac{\partial H}{\partial t} = \nabla(k\nabla T) + Q \quad (2)$$

Back-diffusion model was used for the solidification calculations. Radiation mechanism is the main heat transfer method during the process in the vacuum condition. Triangle surface mesh and tetrahedral volume mesh were used for the calculations. The parameters associated with the simulation process were determined using experimental techniques. Bridgman technique was used for the experimental procedure. The temperature of the hot zone was set to 1600°C. The kinetic parameters associated with the dendritic growth were set according to Kurz-Giovanolla-Trivedi (KGT) model which is described in Equation 3.

$$v = \alpha_2 \Delta T^2 + \alpha_3 \Delta T^3 \quad (3)$$

GTD-111 Ni-based superalloy was used for the experiments in this study.

3- Results and discussions

The volume fraction of the solidified portion of the samples in the Bridgman process is shown in the simulation results at growth rates of 3, 5 and 7 mm/min in Fig.1. The variation of thermal gradient and G.R is plotted as a function of the distance from the chill plate for different growth rates as shown in Fig. 2.

¹ *Corresponding Author, Ph.D Student, School of Metallurgy & Materials Engineering, Iran University of Science and Technology.
Email: ghanbari@iust.ac.ir.

² Professor, School of Metallurgy & Materials Engineering, Iran University of Science and Technology.

³ Professor, School of Metallurgy & Materials Engineering, Iran University of Science and Technology.

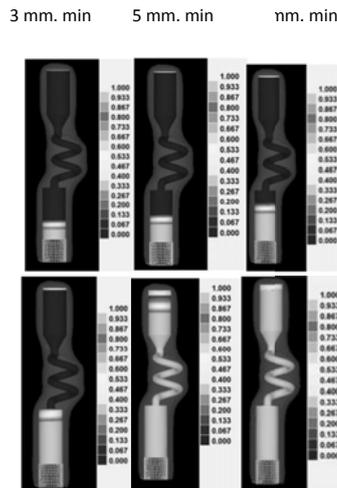


Figure 1 Variation of the solidification during directional solidification

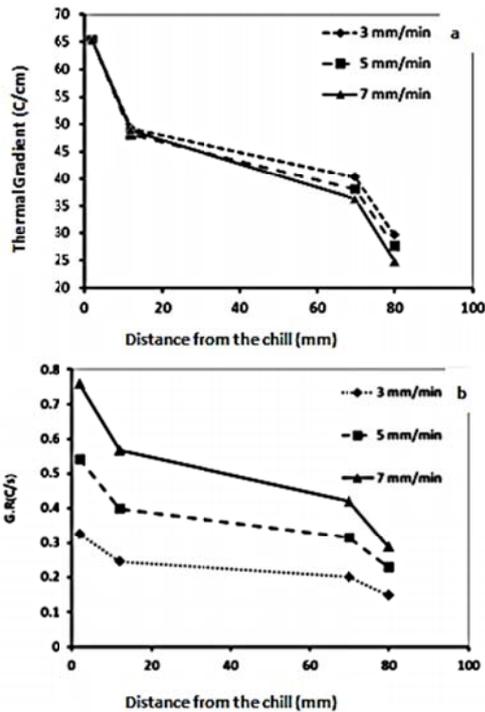


Figure 2 Variation of thermal gradient and G.R parameter vs distance from the chill plate for various growth rates

As seen in Fig. 2, the thermal gradient is decreased by increasing the growth rate and increment of the distance from the chill plate. Based on the calculations done in this study, the value of the f_g in Hunt's equation is plotted as a function of growth rate for different thermal gradients in Fig. 3 which determines the conditions suitable for the formation of stray grains.

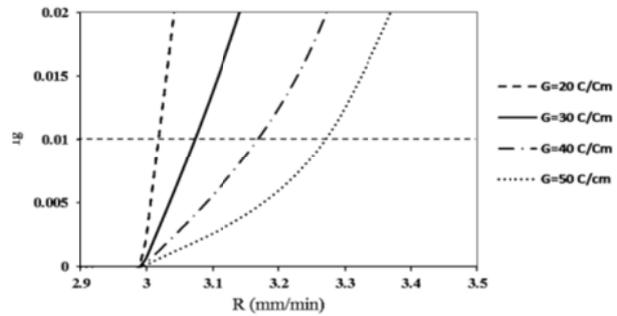


Figure 3 Variation of f_g with growth rate for various thermal gradients

To prevent the formation of equiaxed grains, f_g should be less than 0.01. For example, with the growth rate of 3 mm/min, the thermal gradient should be greater than 20 to 30 °C/cm for GTD-111 superalloy. The results of microstructural simulation using CAFE module are shown in Fig. 4. As seen here, in the conditions described above, the single grain is formed while for the sample with improper growth conditions, stray grains will form.

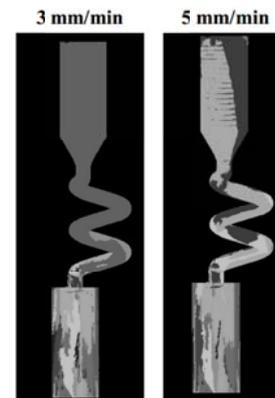


Figure 4 Grain structure of the samples for two different growth rates with thermal gradient of 30 °C/cm

4- Conclusions

To prevent the formation of stray grains in the directional solidification and single crystal growth of GTD-111 in the thermal gradient of 20 to 30 °C the growth rate should be less than 3 mm/min. There is good agreement between the experimental and simulation results in this study.