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Influence of natural and forced gravity conditions during directional columnar solidification

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ABSTRACT

In a recent study, the present authors reported an analysis of a transient process of directional solidification of TiAl alloys in the absence of convection (Battaglioli et al., 2017). The adopted front tracking model, also coupled with indirect methods for predicting columnar to equiaxed transition (CET), showed how the development of different grain regions, namely axial columnar, radial columnar and equiaxed, depends on process parameters such as temperature distribution and applied cooling rates, as well as on properties such as the degree of inoculation of the melt and nucleation undercooling required for equiaxed growth. In this paper, the previous front tracking model is significantly developed, by including the solution of Navier-Stokes equations in order to predict thermal convection in the liquid region as well as in the columnar mush (treated as an isotropic porous medium). This improvement is introduced with the aim to investigate TiAl alloys solidification under different gravity conditions. Accordingly, the simulation setup employed in the study reproduces the one used in experimental campaigns carried out on the MAXUS 9 sounding rocket (microgravity) and on ESA's Large Diameter Centrifuge (hypergravity), within the framework of ESA's GRADECET (Gravity Dependence of CET in TiAl alloys) project. The ability of the model in predicting thermal convection is demonstrated by considering several case studies. Results show that the evolution of fluid flow patterns in the samples depends on the external forces considered, combined to the transient change of axial and radial temperature gradients that occur during the solidification process. A parametric study of the directional solidification process on a centrifuge is performed by changing the value of the centrifuge arm and rotation rate and results are compared to predictions derived from non-dimensional considerations.

1. Introduction

Metallic alloy components for advanced engineering applications, such as aerospace, automotive, and medical industries, are often manufactured by casting processes like investment casting or directional solidification. One of the main advantages of these technologies is the possibility to produce near-net shape components. Nonetheless, in order to produce a component that is free of defects and satisfies given requirements, it is necessary to identify and control important process parameters. In particular, to ensure the attainment of required mechanical properties, it is essential to be able to control the final grain structure of the casting. The development of columnar grains, equiaxed grains, or columnar to equiaxed transition (CET), depends on the transient thermal and fluid flow conditions in the molten alloy. These, in turn, are functions of several interdependent variables, such as imposed temperature gradients, cooling rates, geometric factors and the presence of external forces. For this reason, the choice of process parameters is not straightforward and requires a thorough analysis of the process under consideration. For instance, in the case of directional solidification, specifically defined axial temperature gradients, combined with precise cooling rates (power down mode) or pulling rates (Bridgman mode) are required to ensure the development of the desired grain structure. For example, fully axial columnar grains, desired in industrial applications such as the production of turbine blades, are achieved by using high temperature gradients and low pulling rates [1–3]. On the other hand, several studies show that low temperature gradients combined with high pulling or cooling rates promote the formation of a more extended undercooled region, and hence equiaxed growth [4,5]. Nonetheless, high pulling and cooling rates might induce radial temperature gradients and the development of unwanted radial columnar grains [6–8].

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Nomenclature

b	undercooling exponent
C	dendrite growth coefficient
c_p	specific heat capacity
g	Earth's gravitational acceleration
g_l	liquid fraction
g_s	solid fraction
Gr	Grashof number
h	heat transfer coefficient
k	thermal conductivity
Pe	Péclet number
r	radial coordinate
R_C	centrifuge arm
Re	Reynolds number
Ro	Rossby number
t	time
T	temperature
T_L	liquidus temperature
T_S	solidus temperature
Ta	Taylor number
u	velocity
v_t	dendrite tip growth rate
x	axial coordinate
α	thermal diffusivity
β	coefficient of thermal expansion
μ	dynamic viscosity
ν	kinematic viscosity
ρ	density
ϕ	general variable
ω	centrifuge angular velocity

Subscripts

CV	control volume
dom	computational domain
l	liquid
m	mush
nb	neighbouring CVs
s	solid
samp	sample

In addition to thermal conditions, it is imperative to consider also the effect of external forces which might be present during the solidification process. First of all, unless in the case of microgravity experiments in space, any solidifying alloy is subject to terrestrial gravitational acceleration. This, combined with temperature, density, and composition gradients, induces several phenomena such as convection in the melt, segregation, and buoyancy or sedimentation. For this reason, the influence of terrestrial gravitational field on solidification has been extensively investigated in the literature. Narrowing down to studies that consider directional solidification, different conditions can be investigated, such as thermal stabilizing situations, i.e. upward solidification, or unstabilizing conditions such as in the case of downward solidification. Nonetheless, in both cases predicting the final outcome is not trivial. For example, it has been shown that even in stabilizing conditions, convection may arise due to radial temperature gradients, inducing significant segregation [9–12]. On the other hand strong unsteady convection might lead to a high degree of mixing and reduce segregation [9]. Considering the effect on the development of the grain structure, natural convection modifies the heat fluxes in the melt, affecting temperature gradients and the extent of the undercooled liquid zone. In general, previous studies showed that melt convection has a tendency to promote the occurrence of CET, due both to the reduction of temperature gradients, and to the mechanism of dendrite fragmentation that improves equiaxed nucleation [4,13,14].

Besides terrestrial gravity, additional forces could be related to external accelerations imposed to the mould. One important example is centrifugal casting. This process is often employed since centrifugal forces help mould feeding and filling processes, especially when dealing with lightweight or highly reactive alloys. At the same time, however, centrifugal acceleration influences melt convection. Furthermore, in the case of rotation, the effect of Coriolis acceleration cannot be neglected. For what concerns directional solidification under the influence of centrifugal and Coriolis forces, most studies in the literature focus on crystal growth of semiconductors rather then alloy solidification. A remarkable result was found by Rodot et al. [15,16] when studying the effect of increased gravity obtained by centrifugal force on crystal growth of PbTe and Pb1-xSnxTe. They observed that, for a well defined value of the centrifugal force, the crystal quality and homogeneity were improved, and the segregation profiles were similar to the ones expected in the absence of convection under microgravity. The authors hypothesized that this particular condition was a combined effect of the centrifugal force and the action of Coriolis acceleration. Müller and Weber [17,18] carried out an extensive study, both experimental and numerical, for better understanding the stabilizing effect of centrifugal motion on the convective flow during solidification. From the experiments, the authors observed that for particular acceleration levels, the crystal started to grow without striations, due to a transition from an unsteady to a steady flow. Accordingly, the numerical simulations predicted a transition from an unsteady flow state called I, to a steady flow state II. The authors concluded that the flow pattern in the sample, and hence the enhanced quality of the crystals grown at higher rotation speed, was an effect of Coriolis force, rather than centrifugal force. Lan et al. [19] performed a self-consistent simulation of gradient-freeze crystal growth in a centrifuge and observed that for a horizontal configuration (decreasing temperature with distance form centrifuge axis), the flow speed decreased monotonically with the rotation speed, and as result the unstable flow was suppressed; for a free-swing configuration a condition for a minimum convection was found, where Coriolis force balanced the gravitational ones. Several possible reasons for the minimum in convection were proposed by Wilcox et al. [20], for example due to a balance between buoyancy forces and Coriolis forces, or the occurrence of thermal stability conditions (density gradients parallel to net acceleration vectors). However, predictions based on these criteria did not find a clear correlation with experimental results. It is worth noting that all the previous investigations are focused on crystal growth. On the other hand, to the authors' knowledge, studies on directional solidification of metal alloys in centrifuges are not present in the published literature.

For the reasons highlighted above, it is evident that a full understanding of the effects of both thermal variables and external forces is required in order to predict the grain structure development during a given solidification process and produce high quality castings. With this intent, a recent European project, called GRADECET (GRAvity Dependence of Columnar to Equiaxed Transition in TiAl alloys) has been dedicated to the investigation of the