Journal of Alloys and Compounds 586 (2014) S267–S273

Contents lists available at SciVerse ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jalcom

Numerical modeling of power-down directional solidification process of Ti–46Al–8Nb refractory alloy

A.V. Kartavykh [a,b,*], V.P. Ginkin [c], S.M. Ganina [c]

[a] *National University of Science and Technology "MISIS", Leninsky pr. 4, 119049 Moscow, Russia*
[b] *Technological Institute for Superhard and Novel Carbon Materials (TISNCM), 7a Centralnaya str., 142190 Troitsk, Moscow, Russia*
[c] *Institute for Physics and Power Engineering (IPPE), Bondarenko sq. 1, 249033 Obninsk, Russia*

ARTICLE INFO

Article history:
Available online 22 December 2012

Keywords:
Intermetallics
Crystal growth
Microstructure

ABSTRACT

The work represents a brief outline of developed GIGAN computing code and its application for 2D-description of power-down directional solidification (DS) process applied recently in the course of laboratory R&D of new structural TiAl-based alloys. The temporal temperature field mapping, macro-scale study of melt hydrodynamics, heat-mass transfer, segregation effects, mushy zone evolution and solidification dynamics of TiAl–Nb melt/solid system have been performed numerically for set of DS trials being implemented virtually at different operational regimes and gravity environment. As the example of noteworthy numerical study results, the explanation of centerline peritectic segregation effect in Ti–46Al–8Nb ingots is mentioned, as well as the applied model verification using benchmark DS of TiAl–Nb alloy in microgravity aboard the MAXUS-8 ESA sounding rocket.

1. Introduction

Directionally solidified intermetallic composites offer many advantages for high temperature structural applications, including high strength and excellent creep resistance at elevated temperatures [1]. Ti–46Al–8Nb (at.%) lightweight intermetallic alloy, recently developed within pan-European IMPRESS project, is creep resistant to high temperatures (~1100 K), so being one of the most promising advanced materials for turbine blades of aircraft engines [2]. The developed TiAl–Nb alloy is intended to substitute the contemporary "heavy" nickel superalloys in the new high-effective turbojet design [3]. In contrast to most of TiAl-based alloys, the Ti–46Al–8Nb is characterized by the desired combination of ductility and fracture toughness at ambient temperature with high-temperature strength that, however, require the formation of a special two-phase polycrystalline microstructure of ingots or functional cast items.

The conventional *Bridgman* process is predominantly applied for manufacturing DS turbine blades made of Ni-based superalloys [4,5]. Alongside, for fundamental research of microstructure formation in solidifying Ti–46Al–8Nb, the well-equipped laboratory tube furnaces were applied with power-down principle of thermal gradient operation [6,7]. The applied experimental DS technique could be defined like a sort of vertical gradient freezing (VGF) solidification implemented through the programmable power-down operation of the lateral multi-zone heater coils to obtain required axial temperature profile in solidifying system. DS proceeded upward from the lower "cool" end of the melt column to the upper "hot" one by lowering (decaying with time) the thermal profile with the preset cooling rate at heater coils. The facility contains no moveable parts unlike to the *Bridgman* furnace. Generally, the operating principle of thermal field control and simplified furnace design both improve the flexibility and safety of DS process when compared to the *Bridgman* method, avoiding the application of mechanical units/drives, which run at elevated temperatures, and related disturbing vibrations.

Creation of a uniform, reproducible and balanced alloy microstructure with optimal orientation-dimensional parameters cannot be done without a mathematical modeling of heat-mass exchange in the course of alloy solidification process, and therefore requires the careful support by numerical investigations. Basic numerical approaches for structure modeling in cast and DS alloys have included the Monte Carlo [8], cellular automata [9,10], front tracking [11,12], and phase-field methods [13,14]. Successfully supplementing each other, these methods give a complete enough pattern of multi-scale spatial cast structure formation. However, no applications of these methods are known from the literature for the modeling of microstructure appeared in TiAl-based alloys, perhaps excepting Ref. [15].

The current paper represents briefly the general description of one more mathematical model of multi-component alloy solidification that underlies the developed GIGAN computing code, as

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* Corresponding author at: National University of Science and Technology "MISIS", Leninsky pr. 4, 119049 Moscow, Russia. Tel.: +7 495 5126091; fax: +7 499 7889032.
E-mail addresses: karta@korolev-net.ru, karta@girmet.ru (A.V. Kartavykh).

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http://dx.doi.org/10.1016/j.jallcom.2012.12.063

well as selected examples of its successful applicability for the elaboration of novel TiAl-based structural alloy processing route.

2. Theory/calculation

In the modeled solidifying system a matter can be in the solid, liquid or mushy state which is a mixture of the solid and liquid in different proportions. In vertical DS mushy zone is confined from the bottom by the eutectic temperature T_e (or the solidus temperature for non-eutectic alloys, like TiAl–Nb) and from the top by the liquidus temperature T_{liq} that depends on the concentration of solutes in the melt C_l^i. Choosing the main component that has the largest concentration, let us treat our multicomponent melt as a single-component one. The rest of the components will be regarded as solutes. For binary alloys there is the commonly accepted formula of the linearized liquidus temperature dependence on the admixture concentration: $T_{liq} = T_m + mC_l$. We assume further that the number of solutes is n and they do not interact with one another. Similarly to binary melts let us assume that the dependence of T_{liq} on C_l^i is linearized: $T_{liq} = T_m + \sum_{i=1}^{n} m^i C_l^i$, where m^i are the slopes of the lines of the liquidus hyper-surface intersection with the coordinate planes (on the phase diagram) for the ith solute and the main component (given constants), T_m is the melting temperature of the "pure" material (i.e., for all $C_l^i = 0$). Let us introduce ε_l and ε_s, the volume fractions of the phases in a volume unit of mushy zone. From this statement we shall use the indices l and s to refer to the liquid and solid phase, respectively. The volume fraction of the liquid phase is also referred to as material porosity by definition $\varepsilon_l + \varepsilon_s = 1$. Since the density of the liquid phase ρ_l, and that of solid ρ_s are different, the density of matter in mushy zone will be $\rho = \varepsilon_l\rho_l + \varepsilon_s\rho_s$. Similarly the thermal conductivity coefficient k, the ith solute diffusion coefficient D^i, and the heat capacity c_p in mushy zone are determined: $k = \varepsilon_l k_l + \varepsilon_s k_s, D^i = \varepsilon_l^i D_l^i + \varepsilon_s D_s^i, c_p = \varepsilon_l c_{pl} + \varepsilon_s c_{ps}$.

As usually solute diffusion in the solid phase is neglected, i.e., we assume that $D_s^i = 0$, $D^i = \varepsilon_l^i D_l^i$. On the phase boundary (interface) $C_s^i = k_0^i C_l^i$, where k_0^i is the ith solute distribution coefficient describing the fraction of the ith solute that transforms from liquid into solid during the solidification process. Also we assume the mass transfer at the phase boundary to be instantaneous. Let us introduce the following notation:

$$\mathbf{V} = \varepsilon_l \mathbf{v}_l; p = p_l; h_s = c_{ps}(T - T_e);$$

$$h_l = c_{pl}\ (T - T_e) + L; \langle h \rangle = c_p\ (T - T_e) + \varepsilon_l L;$$

$$\langle C^i \rangle = \varepsilon_l C_l^i + \varepsilon_s C_s^i = (\varepsilon_l + (1 - \varepsilon_l)k_0^i)C_l^i,$$

where $\mathbf{v}_l$ is the true melt flow velocity, $\mathbf{V}$ is the melt seepage velocity in mushy zone, p is the pressure, T is the temperature of the material, h_s is the specific enthalpy of the material in the solid, h_l is the specific enthalpy of the material in the liquid, $\langle h \rangle$ is the specific enthalpy of the material in mushy zone, L is the latent heat of phase transition. Let us assume that the Boussinesq approximation is applicable to the melt flow and the melt density is linearly dependent on the solute temperature and concentration: $\tilde{\rho} = \rho_1 \left[1 - \beta_T(T - T_0) - \sum_{i=1}^{n} \left(\beta_c^i (C_1^i - C_0^i)\right)\right]$, where ρ_l is the melt density at $T = T_0$ and $C_l^i = C_0^i$ (we assume it to be a constant), β_T is the thermal expansion coefficient, β_C^i is the concentration expansion coefficient for the ith solute. Then the heat-mass transfer equations based on the *Navier–Stokes* approach will take the following form:

Equation of motion

$$\rho_l \frac{\partial \mathbf{V}}{\partial t} + \frac{\rho_l}{\varepsilon_l}(\nabla \mathbf{V}) \cdot \mathbf{V} = \nabla \cdot (\mu \nabla \mathbf{V}) - \varepsilon_l \nabla p + \varepsilon_l \tilde{\rho} \vec{g} - \frac{\mu \varepsilon_l}{K}\mathbf{V}, \tag{1}$$

where μ is constant dynamic viscosity.

Equation of continuity

$$\nabla \cdot \mathbf{V} = 0. \tag{2}$$

Energy conservation equation

$$\frac{\partial \rho \langle h \rangle}{\partial t} + \nabla\ (\rho c_p T) \cdot \mathbf{V} - \nabla \cdot (k \nabla T) = 0. \tag{3}$$

Transport equation for the ith solute

$$\frac{\partial \langle C^i \rangle}{\partial t} + \nabla C_l^i \cdot \mathbf{V} - \nabla \cdot (D^i \nabla C_l^i) = 0, \quad i = 1, 2, \ldots n \tag{4}$$

The last term in the equation of motion (1) takes account of the force resisting the melt flow in the porous medium by analogy with *Darcy* law:

$$F = -\frac{\mu \varepsilon_l}{\mathrm{K}}\mathbf{V}, \tag{5}$$

where K is the permeability of the porous medium for fluid flows.

The permeability K depends not only on the porosity ε_l, but also on other non-dimensional characteristics of the porous medium geometry. Numerous attempts have been made to obtain a mathematical description of K for typical porous media by both considering the simplest models and analyzing the experimental data available. All the results obtained so far relate to particular cases and their domain of applicability is rather narrow. The best known is the Kozeny–Carman formula based on the analogy between the porous medium and a system of parallel capillary pipes and expressing permeability in terms of pore specific surface area and porosity. From Ref. [16], for convective heat-mass exchange during binary alloy solidification, the Kozeny–Carman relation for permeability takes the form: $\mathrm{K} = \frac{\lambda_2^2 \varepsilon_l^3}{180\varepsilon_s^2}$, where λ_2 is the secondary dendrite arm spacing in polycrystalline dendrites (empirical value, varies from material to material). In our model we used the same formula.

The system of four Eqs. (1–4) contains five unknown variables $\mathbf{V}$, p, $\langle h \rangle$, C_l, ε_l. So we need one more equation. Let us use an equation describing the dependence of porosity ε_l on the enthalpy $\varepsilon_l = \varepsilon_l(\langle h \rangle)$. This dependence for Ti–46Al–8Nb has been determined from the experiment in paper [17], and is given for solid, mushy and liquid state of the alloy, respectively, by the following formula (6):

$$\varepsilon_l = \begin{cases} 0, & \langle h \rangle \leqslant 0 \\ \frac{c_p^2}{4L^2}\left(\sqrt{1 + \frac{4L\langle h \rangle}{c_p^2 T_{liq}^2}} - 1)\right)^2, & 0 < \langle h \rangle < c_p T_{liq} + L \\ 1, & \langle h \rangle \geqslant L \end{cases}$$

Thus, an explicit expression for the sought closing relation is found. The described model consisting of differential Eqs. (1–4) and relation (6) was realized in the framework of the software package GIGAN developed in IPPE. A complete description of the solving computational GIGAN algorithm can be found in [18]. Before the application to alloy under study, the model was successfully tested and verified using the international benchmark of solidification of eutectic system Sn–Pb, described in [16]. Key thermophysical properties of Ti–46Al–8Nb alloy used in current modeling are pooled in Table 1 that is composed from the data of Refs. [19–21].

For real-time observation of solidification and heat-mass transfer processes within solidifying system, current numerical temperature evolution along the boundaries of calculation domain is necessary to be known as the input data when modeling. Therefore these thermal boundary conditions must be continuously evaluated in the course of DS with the minimal increment of time,