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Combined analytical and numerical front tracking approach to modeling directional solidification of a TiAl-based intermetallic alloy for design of microgravity experiments

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Abstract. A three-step combined analytical and numerical approach to thermal modelling of a two-heater power-down furnace for controlled directional solidification of an intermetallic alloy is proposed. An analytical sensitivity analysis of the thermal model is carried out to show the effect of adiabatic zone length, and both hot-zone and cold-zone heater temperatures, on the initial thermal gradient in the sample and on the length of melt in the adiabatic zone. The subsequent axisymmetric front tracking method (FTM) simulations of directional solidification of a binary intermetallic Ti-46at.%Al alloy show that temperature gradient in the melt declines and velocity of the solid-liquid front increases with time, thus promoting good conditions for a columnar to equiaxed transition. The proposed analytical calculations combined with full-scale numerical FTM simulations provide a convenient and predictive optimization tool for the two-heater power-down furnace design and growth conditions for the future microgravity experiments.

Introduction

The microgravity environment of space and/or free fall conditions offer engineers and scientists a unique opportunity to conduct experiments that erase the complex interactions of gravity-induced and gravity-independent flow, heat and mass transport mechanisms [1].

To realize benefits from materials science in space, design and execution of reduced-gravity experiments must be guided by on-going synergistic theoretical and numerical studies in combination with extensive ground-based experiments and measurements of thermophysical properties. This basis must be established to optimize the pre-flight design and support post-flight analysis. All such aspects of this approach are being pursued in the IMPRESS (Intermetallic Materials Processing in Relation to Earth and Space Solidification) research project, which has a number of scientific and technical objectives that will lead to the creation of advanced prototypes for extreme applications. The selected applications include the development of a novel, low density, highly heat-resistant structural γ -TiAl intermetallic alloy and incorporation of this novel material into aircraft and rotating components under severe conditions, e.g. large 40 cm low-pressure turbine blades for commercial aero-engines [2]. One of the main scientific objectives of the IMPRESS project is quantitative determination and understanding of the fundamental mechanisms that control growth and evolution of grains, including the columnar to equiaxed transition (CET), during solidification of γ -TiAl intermetallic alloys. To achieve this challenging objective, which will ultimately lead to novel casting processes for defect-free turbine blades with tailor-made properties, controlled directional solidification reduced-gravity experiments have to be designed and precisely executed.

There are three basic techniques of accomplishing controlled directional solidification: i) Bridgman-Stockbarger growth, ii) the gradient freeze method and iii) the power down technique. After extensive theoretical and numerical analysis carried out by a dedicated IMPRESS team, the power down technique has been selected for a realization of the sounding rocket (MAXUS-8) furnace. This paper focuses on a *two-heater power-down furnace* concept and associated design methodology combining numerical front tracking method (FTM) and an analytical approach. This furnace case was being actively investigated by the IMPRESS team, prior to being superseded by a *three in-line heater power-down variant* [3]. Sensitivity analyses using the authors' thermal model were carried out to show the effect of adiabatic zone length, and hot-zone and cold-zone heater temperatures, on initial thermal gradient in the sample and length of melt in the adiabatic zone. The subsequent detailed FTM simulations showed a temporal decline of temperature gradient in the melt and increasing velocity of solid-liquid front, promoting good conditions for the CET. The proposed full-scale numerical FTM simulations combined with analytical calculations provide a convenient and predictive optimization tool for the power-down two-heater furnace design and growth conditions.

Proposed approach to thermal modeling of a power-down two-heater furnace

The methodology to design the power-down two-heater furnace and specify growth conditions proposed in this paper consists of three steps: i) evaluation of average heat transfer coefficients in the hot and cold zones of the furnace, based on the Fu and Wilcox model [4]; ii) one-dimensional Naumann analytical calculations of initial thermal gradient in the sample and length of melt in the adiabatic zone of the furnace [5], iii) FTM numerical simulations of a columnar dendritic growth and evaluations of CET conditions [6,7,8]. Figure 1 outlines the proposed combined design approach with all inputs and outputs.

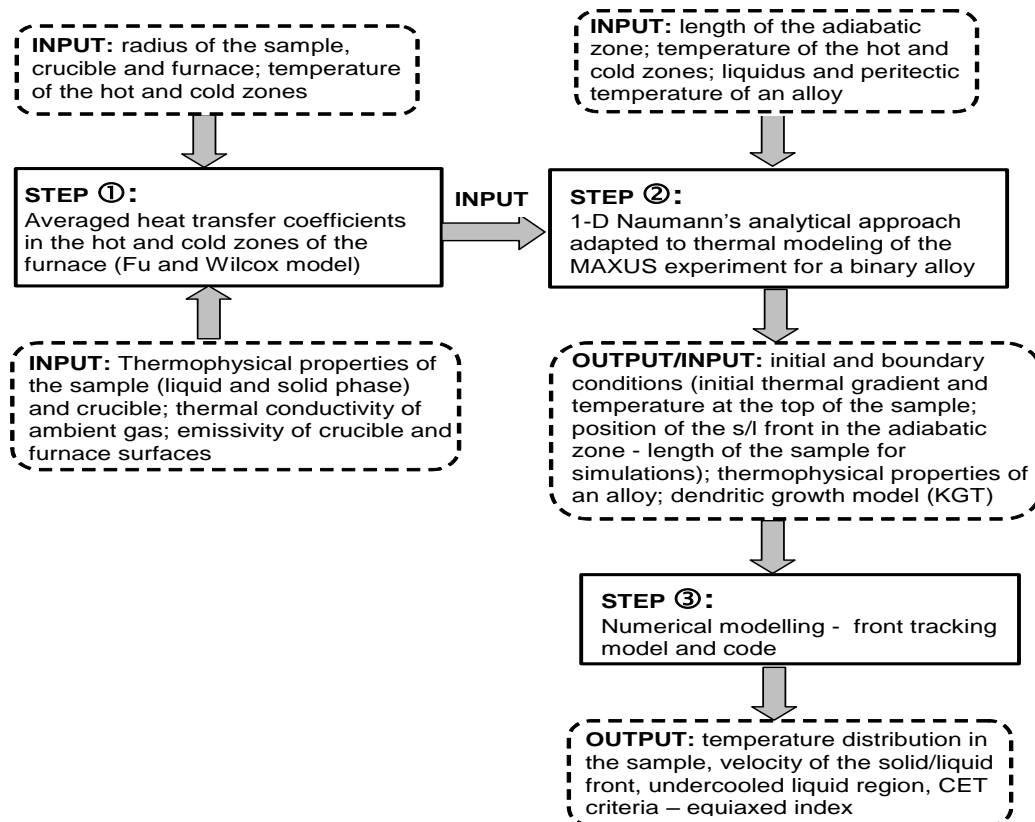


Fig 1. Combined analytical and FTM numerical approach to thermal modeling of the power-down two-heater furnace concept.

To calculate the heat transfer coefficients in hot and cold zones of the power-down two-heater furnace (1st step) two sets of input data are necessary. The first set consists of the following dimensions: 4 mm radius of alloy sample, 6 mm external radius of crucible, 7 mm external radius of surrounding cartridge, 10 mm radius of furnace bore, with temperature of heaters ranging from 1200 to 1700°C. The second set comprises selected thermophysical properties of a Ti-46at.%Al alloy sample, dense yttria (Y₂O₃) crucible, tantalum (Ta) cartridge, argon (Ar) as an ambient gas and diffuse and gray surfaces of heaters. Thermal conductivities are assumed to be as follows: $k_{Y_2O_3} = 4.2 - 3.6$ [W/m·K]; $k_{Ar} = 0.058 - 0.067$ [W/m·K]; $k_{Ta} = 57.5$ [W/m·K]. Thermal emissivities of heaters and cartridge surfaces are equal to 0.45 or 0.30 and 0.5, respectively.

Average computed heat transfer coefficient (H.T.C.) at the surfaces of hot and cold zones of the two-heater furnace as a function of heater temperature, for two values of their emissivity, are plotted in Fig. 2 along with derived linear correlations.

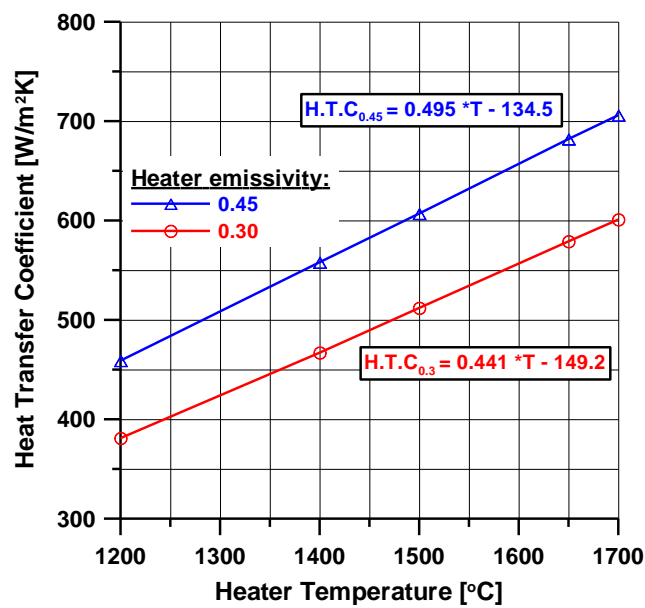


Fig. 2. Average heat transfer coefficients (H.T.C.) at surfaces of hot and cold zones of the power-down two-heater furnace for two values of emissivity as a function of heater temperature.

Initial temperature gradient in the melt, position of the solid-liquid interface in the adiabatic zone and temperature of the melt at the top of the adiabatic region are next determined with the help of one-dimensional Naumann analytical model (2nd step) by using input data containing the heat transfer coefficients (1st step) and temperature of the hot and cold zones equal to, respectively 1700°C or 1650°C or 1600°C and 1400°C or 1480°C, length of the adiabatic zone between 2 and 5 cm and selected thermophysical properties of the Ti-46at.%Al alloy including liquidus and peritectic temperature.

The effect of hot-zone heater temperature on the initial thermal gradient in the alloy sample is depicted in Fig. 3a. In this case the length of the adiabatic zone and cold-zone temperature are equal to 5 cm and 1480°C, respectively. It may be seen that it is possible to obtain a thermal gradient (≈ 40 K/cm) in the adiabatic zone if temperature of the hot-zone heater is equal to 1600°C. Note that a position of the solid/liquid (s/l) front (liquidus T_{liq}) is within the adiabatic zone and thermal gradients in the melt (G_L) and solid phase (G_S) are almost equal. A complete sensitivity analysis with the hot-zone heater temperature set at 1700°C is presented in Fig. 3b. An adiabatic zone length of 5 cm, hot-zone and cold-zone heaters temperatures of 1600°C and 1480°C, respectively, were

chosen as input for subsequent detailed FTM simulations in the 3rd step of the proposed approach: initial thermal gradient in the sample is 20 K/cm and the length of the melt in the sample is 3 cm.

The FTM model and code [6,7] developed within CETSOL, a project of the ESA Microgravity Application Promotion programme, was extended to an axisymmetric case of a cylindrical sample. This fixed grid model can track non-equilibrium columnar growth employing laws of dendritic tip kinetics like the Kurz-Giovanola-Trivedi (KGT) one [9] with a newly estimated value of the stability parameter σ^* . Based on recent measurements of crystal-melt surface energy anisotropy strength of aluminium alloys, dendritic tip stability parameters for these alloys were estimated [10]. A similar approach can be used for γ -TiAl intermetallic alloys if their crystal-melt surface energy anisotropy strength will be measured or calculated. However, we can assume that the stability parameter of TiAl intermetallic alloys should be at least twice the commonly used value 0.0253.

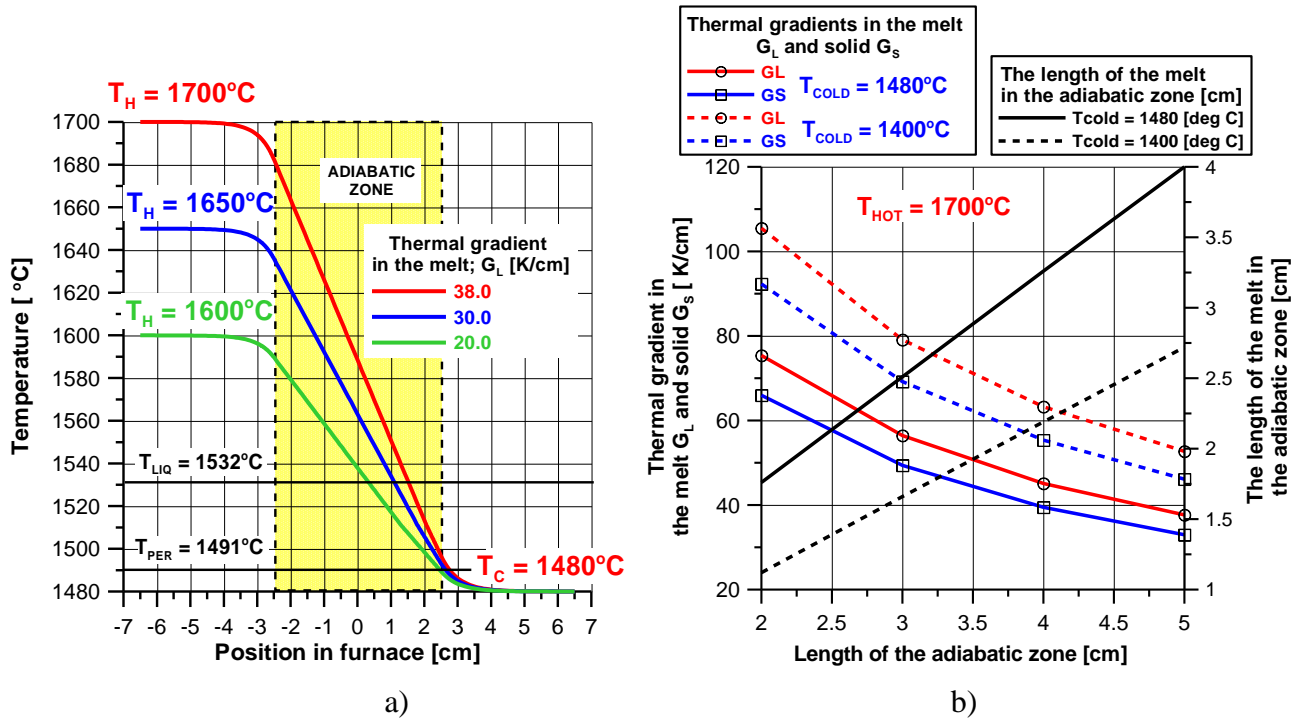


Fig. 3. One-dimensional Naumann analytical calculations of initial thermal gradient in the sample and length of the melt in the adiabatic zone of the furnace: a) effect of hot-zone heater temperature; b) effect of length of the adiabatic zone and cold-zone heater temperature (1480 or 1400°C); hot-zone heater temperature is equal to 1700°C.

The KGT-predicted variations of dendrite tip velocity V_{tip} with solutal undercooling ΔT_c , for the Ti-46at.%Al alloy and two values of stability parameter $\sigma^* = 0.0253$ and 0.0506 , used in FTM simulations are presented in Fig. 4. These predictions are fitted to the following relationship:

$$V_{tip} = A (\Delta T_c)^n \quad (1)$$

where A [$\text{cm s}^{-1} \text{K}^{-n}$] and n are fitting parameters, the values of which are shown in the Fig. 4.

The following thermophysical properties of the Ti-46at%Al binary alloy are used in analytical and FTM calculations: diffusivity of solute in liquid $D_L = 2.8 \cdot 10^{-9}$ [m^2/s]; the Gibbs-Thomson coefficient $\Gamma = 1.5 \cdot 10^{-7}$ [mK]; the partition coefficient $k_0 = 0.917$; the liquidus slope: $m = -12.5$ [K/at\%]; the melting point of Ti 1670 [$^\circ\text{C}$]; liquidus 1532 [$^\circ\text{C}$]; peritectic 1491 [$^\circ\text{C}$]; thermal

conductivity in liquid $k_{liq} = 19.5$ [W/mK] and in solid phases $k_{sol} = 22.8$ [W/mK] (note almost equal values); specific heat of liquid $c_{pliq} = 1040$ [J/kgK] and solid phase $c_{psol} = 860$ [J/kgK]; density of solid and liquid phase $\rho = 3850$ [kg/m³]; latent heat of fusion $H_f = 411$ [kJ/kg].

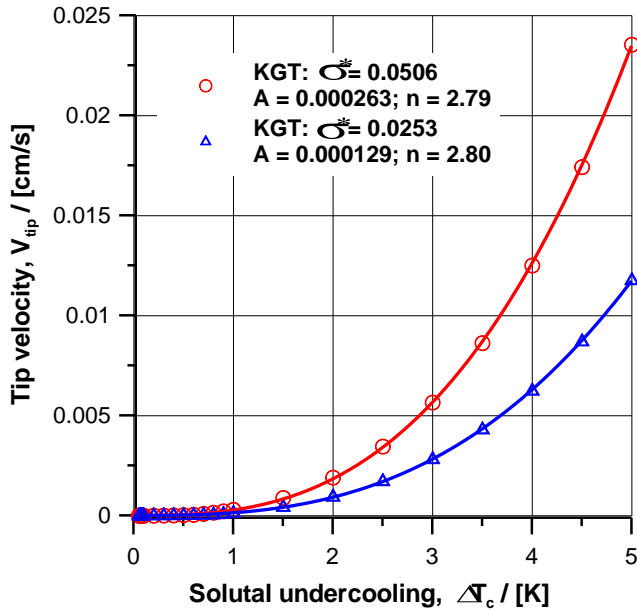


Fig. 4. The KGT-predicted variations of dendrite tip velocity V_{tip} with solutal undercooling ΔT_c .

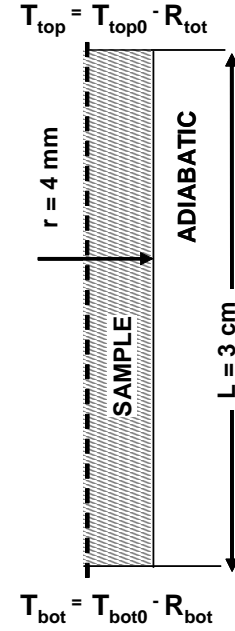


Fig. 5. The Schematic diagram, geometric definitions and computational boundary conditions of a simplified axisymmetric FTM model for the vertical power-down two-heater growth configuration.

Numerical FTM results

In this paper simplified axisymmetric FTM model, as depicted in Fig. 5, is used to model a vertical power-down two-heater growth. Cooling rates at the top and bottom of a sample are calculated using a similar procedure derived for a thermal model of the ARTEX (ARtemis on TEXus) furnace [11]. The computational boundary conditions are summarized below:

- initial gradient in the melt: $G_{L0} = 20$ K/cm,
- initial cooling rate at the top of a sample: $R_{init_top} = G_{L0} \cdot V_{tip} = 0.12$ K/s,
- cooling rate at the bottom of a sample: $R_{bot} = \rho H_f \cdot V_{tip}^2 / k_{sol} + (k_{liq}/k_{sol}) \cdot G_{L0} \cdot V_{tip} = 0.32$ K/s,
- initial temperature at the bottom of a sample: $T_{bot0} = T_{liq} = 1532^\circ\text{C}$
- initial temperature at the top of a sample: $T_{top0} = T_{bot0} + G_{L0} \cdot L = 1592^\circ\text{C}$
- time needed to establish steady-state G_L and V_{tip} in the sample: $t_{steady} = 100$ s
- cooling rate at the top of a sample after 100 s: $R_{top} = R_{bot}$

At the initial stage the lower and upper surface of the sample were cooled with different cooling rates, 0.12 K/s and 0.32 K/s respectively. After the initial 100 seconds the model needed to establish steady-state conditions ($G \approx 25$ [K/cm] and $V \approx 0.006$ [cm/s] – see Fig. 6a), the cooling rate of the upper surface is increased to 0.32 [K/s]. As a result, the temperature gradient drops, velocity of solid-liquid front increases (see Fig. 6a), promoting good conditions for the CET at or before 270 s (see a peak of the equiaxed index [8] in Fig. 6b).

Concluding remarks

The proposed full-scale numerical FTM simulations combined with analytical calculations provide a convenient and useful optimization tool for the power-down two-heater furnace design and growth conditions including the CET. However, once validated and/or verified, the approach developed in this work is generally applicable to a number of solidification processes and furnaces.

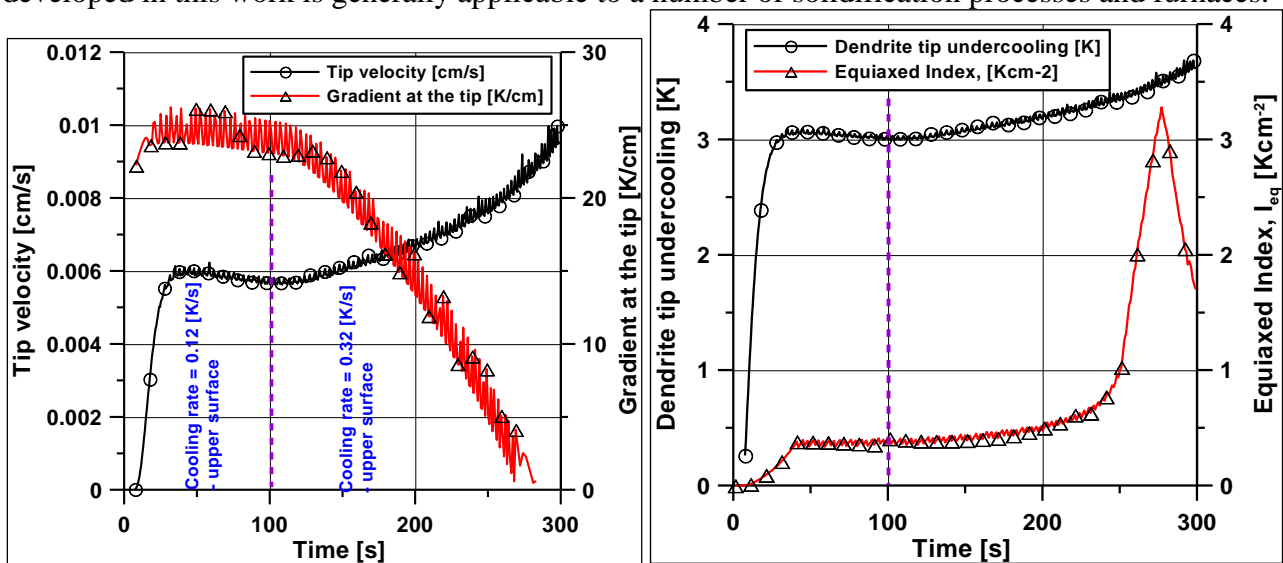


Fig. 6. FTM numerical simulation: a) a dendritic tip velocity and gradient at the tip; b) an equiaxed index and dendrite tip undercooling

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