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Phase-field modelling of $\beta$(Ti) solidification in Ti-45at.%Al: columnar dendrite growth at various gravity levels

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Abstract. The effect of solutal convection on the solidification of $\gamma$ titanium aluminides, specifically on $\beta$(Ti) dendrite growth, is not well known. With the aim of supporting directional solidification experiments under hyper-gravity using a large diameter centrifuge, 2D-phase field simulations of $\beta$(Ti) dendrite growth have been performed for the binary alloy Ti-45at.%Al and various gravity scenarios. Both, the direction and magnitude of the gravity vector were varied systematically in order to reveal the subtle interplay between the convective flow pattern and mushy zone characteristics. In this presentation, gravity effects are discussed for early dendrite growth. For selected cases the evolution on longer timescales is also analysed and oscillatory modes leading to dynamically stable steady state growth are outlined. In a dedicated simulation series forced flow is superimposed, as to mimic thermally driven fluid flow expected to establish on the macroscopic scale (sample size) in the centrifugal experiments. Above a certain threshold this flow turns dominant and precludes solutally driven convective effects.

1. Introduction
The motivation of this study is to reveal convective effects on the characteristics of the mushy zone during directional solidification of bcc $\beta$(Ti) dendrites in hyper-gravity conditions. Such conditions commonly occur during centrifugal casting of near-net shape parts from titanium aluminides (e.g. Ti-45at.%Al) but may be explored more systematically by means of solidification experiments inside ESAs large diameter centrifuge (LDC). In order to guide experiment design and evaluation phase, field simulations were performed for different hyper-g scenarios, focusing on columnar growth of $\beta$(Ti) dendrites as function of the gravity vector $\vec{g}$. Both, the magnitude and direction of $\vec{g}$ were varied within experimentally feasible limits. This means that $\vec{g}$ is either parallel or anti-parallel to the direction of solidification ranging from 0 to $+20\vec{g}$ (parallel) and from 0 to $-20\vec{g}$ (anti-parallel) respectively. In a dedicated simulation series the effect of additional lateral forced flow was investigated for the case of $-17\vec{g}$. Previous work on gravity effects on the solidification behavior of an Al-Cu alloy has been reported based on simulations [1, 2, 3] and based on experiments for a Pb-Sn alloy [4]. These studies showed that gravity impacts on the characteristics of the mushy zone; the primary dendrite arm spacing decreases for specific fluid flow configurations that promote growth of tertiary arms while inhibiting growth of primary dendrite tips through advection of solute.
2. Model description
The phase field model coupled to melt flow that was used in the present work is described in [1, 5]. The simulations are restricted to two dimensions and to early $\beta$(Ti) dendrite growth, e.g. to time periods that are just long enough to allow reaching steady state growth. The partial differential equations for melt flow are solved on a grid with grid spacing twice bigger than that for concentration and phase field, a method suggested by Beckermann [6]. In order to calculate the advection term, the flow velocity is projected on the finer grid using linear interpolation. This method allows speeding up the computations of the complete system by a factor of five for the simulations shown in this paper. In this study only the gravity vector $\vec{g}$ is changed, both in magnitude and direction, while the solidification parameters and other numerical parameters are kept constant. The materials properties for the alloy Ti-45at.%Al are summarized in Table 1, the linear coefficient of density change has been evaluated from numerical calculations by Lopis [7] and the viscosity has been evaluated from experiments by Wunderlich [8]. The temperature dependence of density has been neglected. Directional solidification is modeled by imposing a fixed temperature gradient in $z$-direction $G_z = 120 \text{ K/cm}$ and a cooling rate $r=0.3 \text{ K/s}$, corresponding to a pulling speed of $v_w = 25 \mu\text{m/s}$. The simulations are performed in a rectangular domain of $960\mu\text{m} \times 450\mu\text{m}$, height and width, respectively, starting with a spherical seed at the bottom of the calculation domain, its width defining the initial spacing. Boundary conditions are periodic in $x$-direction. For the concentration field the top boundary is treated with a fixed concentration and the bottom boundary is isolated. Flow is constrained to be parallel to top and bottom boundaries and a non-slip condition is used at the solid-liquid interface. This choice of boundary conditions mimics a situation in which the melt in the far field above the mush would be perfectly mixed (by convection). The phase field parameters are adjusted using the solution of the dendrite tip operating point from the KGT model [9] for the case of directional solidification under purely diffusive conditions ($\vec{g}=0$) and steady state growth. A careful calibration of the interface thickness ($\delta = 1.2 \mu\text{m}$) and phase field mobility ($\mu_{sl} = 2 \cdot 10^{-2} \text{ cm}^4/\text{J/s}$) were performed to ensure convergence of the steady state solutions of tip radius and tip undercooling to KGT solutions.

**Table 1. Physical and numerical parameters used in our simulations**

| Parameter                                      | Value              | Reference |
|------------------------------------------------|--------------------|-----------|
| Density (liquid) ($\rho$)                      | $3.7 \cdot 10^6 \text{ g/m}^3$ | [7]       |
| Density variation ($\partial \rho/\partial c$)  | $1.77 \cdot 10^4 \text{ g/m}^3/\text{at\%}$ | [7]       |
| Kinematic viscosity ($\nu$)                    | $1.89 \cdot 10^{-6} \text{ m}^2/\text{s}$ | [8]       |
| Liquidus slope ($m_l$)                         | $-11.268 \text{ K/at\%}$ | [10]      |
| Partition coefficient ($k_{Al}$)               | 0.9                | [10]      |
| Liquid diffusivity ($D_l$)                     | $3 \cdot 10^{-9} \text{ m}^2/\text{s}$ | [11]      |
| Interfacial energy ($\sigma_{sl}$)             | 0.1                | [12]      |

3. Simulation results
In Ti-45at.%Al, convective flow is driven by local melt density changes caused by the weak segregation of the lighter element Al. The simulation results are presented below for two distinct cases: (I) $\vec{g}$ is aligned parallel to the growth direction and hence aluminum-lean liquid is transported downwards the dendrite tips and (II) $\vec{g}$ is aligned opposite to the growth direction and hence aluminum-rich liquid is rising from the mush, flowing upwards along the dendrite stem and tip. For each case, the growth velocity ($v$) and the average melt flow velocity ($u$) are evaluated and displayed as function of time. The average melt flow velocity was obtained
by summation of the z-component of the velocity along each column of the domain divided by the number of liquid cells in each column. The growth velocity refers to the tip velocity of the longest dendrite in the array. Snapshots of the concentration field and the flow field at different selected time are also included. Case III is expanding the scenario (II) by including an additional forced flow in lateral direction.

3.1. Case I : $\vec{g}$ parallel to the growth direction and microgravity

Figure 1 displays the dendrite evolution in $0\vec{g}$, $1\vec{g}$, $5\vec{g}$ and $15\vec{g}$. A longer time is simulated for microgravity as to verify that steady state is reached. Indeed one can see that it is reached after a damped oscillation at about 100s, the growth velocity converging to the pulling speed represented with a red dashed line. When increasing gravity the convection rolls feed Al-lean liquid to the dendrite tip region, such that one would expect the central dendrite to grow faster, however this effect is rather weak and the length of the central dendrite or the mushy zone is virtually independent from the magnitude of gravity. More pronounced secondary arms develop, which indicates that the flow amplifies the side branching instability. Furthermore, tip splitting of the central dendrite is observed at $15\vec{g}$. The flow velocity increases with gravity but the averaged up- and downward flow velocity remains below the growth velocity. The growth velocity reaches the pulling speed at around 100s, being only slightly affected by the gravity magnitude.

3.2. Case II : $\vec{g}$ opposite to the growth direction

The snapshots and velocity profiles in figure 2 display dendrite growth configurations after solidification onset along with the corresponding flow patterns for different magnitudes of $\vec{g}$ aligned opposite to the growth direction. For this case, the convective flow and the response of the mushy zone are qualitatively different from case I. One can observe the following effects; first, two convection rolls form on each side of the dominant primary dendrite, now with upward flow on both sides of the tip. With increasing magnitude of the gravity vector $\vec{g}$ the initially dominant single dendrite tip grows less fast, being fed with Al-rich melt by upward flow. In the downward flow regions Al-lean melt is advected and correspondingly tertiary dendrite arms grow faster until they become primary dendrites, eventually leading to a decrease of the dendrite spacing. The average flow velocity in the convection rolls increases with gravity. The flow pattern is symmetric, relative to the central primary dendrite for $-1\vec{g}$. The symmetry of the flow pattern is altered at high $\vec{g}$ because the primary spacing is severely reduced and the convection pattern changes in response to the increased number of primary dendrites. Local tip splitting events are also detected. The solidification dynamics shows the following peculiarities, as can be inferred from the average flow velocity profiles and the growth velocity profiles in figure 2, for the lowest gravity ($-1\vec{g}$), the flow velocity is always lower than the dendrite growth velocity and hence dendrite characteristics are only slightly affected. At 100s the growth velocity reaches the pulling speed, e.g. steady state. For $-7\vec{g}$, between 0 and 10s the central dendrite remains dominant but is slowed down by the upward flow. Between 10 and 18 s the quick growth of the tertiary dendrite arm on the right side of the domain in response to the downward flow in this area leads to an increase of the growth velocity. In fact, one can state that the oscillatory behavior of the growth velocity for $t > 10$ s is due to the competition between the different dendrites and their interaction with flow. Finally a dynamic steady state is reached at about $t=60$ s with permanent oscillations of the dendritic front kinetics. This behavior is also observed for higher magnitudes or $\vec{g}$ eventually with shorter periods of the oscillations and with more frequent tip splitting events.
Figure 1. Dendrite growth in Ti-45at.%Al as function of time for case I with the gravity vector oriented parallel to the growth direction. The plots show the growth velocity and the average flow velocity for different magnitudes of $\vec{g}$, black solid line dendrite tip velocity, black dashed line maximal flow $z$-velocity, red dashed line pulling speed. The inserted snapshots display concentration and flow maps.

3.3. Case III: $\vec{g}$ opposite to the growth direction and forced lateral flow

The snapshots in figure 3 display dendrite growth and flow configurations after 10 seconds of solidification under $-17 \vec{g}$ and an additional lateral flow imposed along the x-axis by applying a pressure difference of $\Delta p = 0.1, 1$ and $2$ mPa, respectively. The simulation parameters are the same as before except for the calculation domain that is 600$\mu$m high and 450$\mu$m wide. For $\Delta p = 0.1$ mPa, one can observe that the lateral flow is weaker than the flow driven by solutal convection and hence little impact on the dendrite growth kinetics and morphology is seen. With increasing $\Delta p$ the lateral flow becomes gradually more dominant and precludes the effects of the gravity driven solutal convection. Spacing refinement through excessive growth of tertiary arms is no longer operative. Instead one can observe that the secondary arms of the central dendrite are growing preferentially into the flow, a phenomenon that has been observed many times in experiments [13, 14] and simulations [6]. Nevertheless, the lateral flow velocity has to be several times bigger than the convective flow velocity to induce severe changes of the dendritic morphology. For the present case the threshold value of the lateral flow velocity above which convective effects may be neglected ranges at about twice the maximum velocity in the
convection rolls at $-17\vec{g}$.

4. Summary and conclusion
Phase field simulations were used to investigate the early growth of $\beta$(Ti) dendrites in a directional solidification setup, taking into account the melt convection driven by solutal buoyancy for various hyper-gravity scenarios. The results show distinct effects of gravity on the solidification dynamics and the resulting morphology of the mushy zone, depending on the direction of the gravity vector. For the gravity vector parallel to the growth direction the flow pattern behaves stable and the magnitude of the average flow velocity parallel to the growth direction is always below the pulling speed in the experimentally accessible range ($15\vec{g}$). Consequently, there is only a weak effect on the mushy zone characteristic. The most significant impact of convective flow on the columnar mushy zone is observed if the growth direction is opposite to the $\vec{g}$-vector. In this case, the primary dendrite spacing decrease with increasing magnitude of $\vec{g}$ because flow and solute advection greatly favour the development of tertiary arms into new primary arms. This is due to the fact that the flow pattern becomes unstable, evolves

![Figure 2](image-url)

**Figure 2.** Dendrite growth in Ti-45at.%Al as function of time for case II with the gravity vector opposite to the growth direction. The plots show the growth velocity and the average flow velocity for different magnitudes of $\vec{g}$; black solid line dendrite tip velocity, black dashed line maximal flow z-velocity, red dashed line pulling speed. The inserted snapshots display concentration and flow maps.
on larger length scales and thus results in higher flow velocities. These effects are precluded, if lateral flow is strong, e.g. several times stronger than convective flow. For the analysis of centrifugal experiments it is therefore mandatory to verify the transport rates associated with macroscopic flow in the sample and to use the results as an input to meso and microscale models. As discussed in [1] the present simulation results are 2D and not independent from the computational domain size and must be regarded as qualitative results so far. However, they will be used for the calibration of a mesoscale model [15] that will address the 3D problem in future.

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References
[1] Steinbach I 2009 Acta. Mat. 57 2640
[2] Apel M and Diepers H-J MCWASP XI Proceedings 505
[3] Diepers H J and Steinbach I 2006 Material Science Forum 508 145
[4] Bataille C C Grugel R N Hmelo A B and Wang T G 1994 Metal Trans A 25 865
[5] Beckermann C Diepers H-J Steinbach I Karma A Tong X 1999 J. Comp. Phys. 154 468
[6] Lu Y Beckermann C and Ramirez J C 2005 Journal of crystal growth 280 320
[7] Lopis A S Computational simulation of molten titanium-aluminum metal and alloys (available at http://www.mintek.co.za/Pyromet/Files/2010Lopis.pdf).
[8] Wunderlich R 2008 High Temperature Materials and Processes 27 401
[9] Kurz W Giovonola and B Trivedi R 1986 Acta Mat. 34 823
[10] Witusiewicz V T Bondar A A Hecht U Rex S and Ya T 2008 Alloy Compd. 465 64
[11] Binder K and Kargl F 2012 Gradeiet Meeting Budapest 4 Unpublished
[12] Eiken J Apel M Witusiewicz V T Zollinger J and Hecht U 2009 J. Phys.: Cond. Mat. 21 464104.
[13] Shevchenko N Eckert S Boden S and Gerbeth G 2012 IOP Conf. Ser.: Mater. Sci. Eng. 33 012035
[14] Okamoto T Kishitate K and Besho I 1975 J. of Crys. Growth 29 131
[15] Založnik M Viardin A Combeau H and Apel M 2014 submitted to ICASP 4 Proceedings