Title	Analysis of a Microgravity Solidification Experiment for Columnar to Equiaxed Transitions with Modeling Results
Authors(s)	McFadden, Shaun, Browne, David J., Sturz, Laszlo, et al.
Publication date	2010-05
Publication information	McFadden, Shaun, David J. Browne, Laszlo Sturz, and et al. "Analysis of a Microgravity Solidification Experiment for Columnar to Equiaxed Transitions with Modeling Results" 649 (May, 2010).
Publisher	Trans Tech Publications
Item record/more information	http://hdl.handle.net/10197/4701
Publisher's version (DOI)	10.4028/www.scientific.net/MSF.649.361

Downloaded 2023-04-07T10:52:29Z

The UCD community has made this article openly available. Please share how this access benefits you. Your story matters! (@ucd_oa)

© Some rights reserved. For more information

Analysis of a Microgravity Solidification Experiment for Columnar to Equiaxed Transitions with Modeling Results

Shaun McFadden^{1, a}, David J. Browne^{1, b}, Laszlo Sturz^{2, c} and Gerhard Zimmermann^{2, d}

¹School of Electrical, Electronic, and Mechanical Engineering, University College Dublin, Ireland

²ACCESS eV, Aachen, Germany

^ashaun.mcfadden@ucd.ie, ^bdavid.browne@ucd.ie, ^cL.sturz@access.rwth-aachen.de,

^dg.zimmermann@access.rwth-aachen.de

Keywords: solidification modeling, columnar equiaxed transition

Abstract. This paper studies the Columnar to Equiaxed Transition (CET) in an Al-7wt%Si binary alloy with and without Al-Ti-B grain refiner. A microgravity experiment was designed to produce a CET in this alloy system. The experiment was flown onboard the MAXUS-7 sounding rocket platform, which achieved twelve minutes of microgravity. Examples of CET were successfully produced during the unmanned flight. Temperature data were recorded from thermocouples in the crucible walls of the furnace. Post-mortem material characterization of the grain structure was also performed. Subsequently a model of the furnace, which used a front-tracking model of solidification and an inverse heat calculation method, was developed. In this paper, results from the model are compared to the experimental findings; agreement is found with the CET predictions. The results from the model are then used to compare findings with the CET criterion of Hunt from the literature. Agreement is found between the model predictions and the Hunt criterion.

Introduction

This paper presents a study on the Columnar to Equiaxed Transition (CET). A CET experiment was designed for an Al-7wt%Si alloy. This experimental apparatus was launched on the MAXUS-7 sounding rocket. Thus, the experiment was performed under microgravity conditions during the free fall in the MAXUS-7's flight trajectory. Under microgravity conditions, the effects of gravity on fluid flow are greatly suppressed. Therefore, it is assumed that, under microgravity conditions, liquid-solid phase transformations are controlled by diffusion. Thus, microgravity experimentation provides a unique environment for studying fundamental diffusion-controlled solidification of alloys.

This paper explains details of analysis performed on the microgravity experiments with assistance from a numerical model of the furnace. The model used a front-tracking method to calculate the thermal conditions and solidification macrostructure that evolved during solidification.

Essential Background Literature

Experimental Details and Results. The Swedish Space Corporation together with the European Space Agency and EADS-Astrium launched the MAXUS-7 sounding rocket from the ESRANGE site on 2 May 2006 [1]. A solidification experiment onboard this platform was given the acronym MACE (standing for Metallic Alloys for Columnar Equiaxed solidification). Three separate scenarios were performed in the experiment: MACE A, MACE B, and MACE C. All scenarios involved the binary alloy Al-7wt%Si; however, MACE B included an Al-Ti-B grain refiner. The details and main results from all three experimental scenarios have been published [2]. After post-mortem analysis of the samples, it was shown that MACE A and MACE B produced a CET in the macrostructure. Further analysis and results of the CET from MACE A and MACE B are published in [3]. For our purposes, within this paper, only MACE A and MACE B are considered.

Modeling Details. To facilitate further analysis of the samples, a model of the MACE furnace was developed [4]. This model used the front tracking method of McFadden and Browne [5] to simulate the evolving macrostructure during the liquid-to-solid transformation. An inverse heat transfer method was used to reconstruct the thermal conditions in the model. Preliminary results from this model along with explanation of the main adjustable parameters within the model are presented elsewhere [4]. The calculated temperatures agreed well with measured temperatures. Further post-processing of the modeling results are presented here.

Results (Experimental versus the Model)

Fig. 1 shows the results of the simulated 2-D macrographs from the front tracking model [4] and the experimental macrographs from references [2,3]. MACE A is shown on the left and MACE B is shown on the right. The simulation from MACE A used 100 initial seeds ($N_o=100$), whereas, the MACE B simulation used 500 ($N_o=500$). The seed positions were randomly distributed throughout the initial liquid with a uniform probability. The undercooling required for seed initiation (or nucleation) was also random and was based on a log-normal probability distribution of the seed particles' diameters.

Fig. 1: MACE A and MACE B grain structure comparisons

Fig. 2: Grain area data along the longitudinal length of the sample (from experiment results)

In the case of MACE B, the CET position in the experimental results was not clear to the eye. Statistical post-processing of the macrograph showed that a CET existed. As demonstrated in Sturz et al. [2], the plot of average grain area along the longitudinal section of the sample revealed the CET position. The average grain area was relatively large for the columnar region and relatively smaller for the equiaxed region. Fig. 2 shows the measured grain areas in the longitudinal section, with error bars, for MACE A (i) and MACE B (ii). The CET in MACE A occurred at around position 147.5 mm and in MACE B, it occurred at around 132.5 mm. The columnar zone in MACE B was quite mixed between equiaxed and columnar grains, hence the difficulty in observing the transition.

Fig. 3: Grain area data along the longitudinal length of the sample (from model results)

The modeling results show clear CET positions. Calculating the grain area along the length of the simulated results showed that when the number of seeds (N_0) was 100, the CET was observed at 143 mm - fig. 3(i). When the number of seeds was increased to 500 in the simulation, the CET occurred at approximately 137 mm - fig. 3(ii). The number of seeds used in the simulations was approximated. The 2D seed densities used in the simulations are 23.1 cm^{-2} for MACE A and 115.7 cm^{-2} for MACE B. A 3D to 2D conversion of seed density data is difficult to interpret and was not attempted. The seed data used in the simulation was selected to demonstrate the qualitative effect of increasing the number of seeds (that is, the effect of adding a grain refiner). Agreements with the measured CET positions are reasonable. Grain area values in the columnar region vary considerably between the model predictions and the measured values. This discrepancy is due to the 2D nature of the model and the lack of crystallographic orientation information in the front tracking model. In reality, the columnar grains are 3D and may have some crystallographic misalignment that allows the crystals to grow at an angle to the 2D plane [6]. Columnar misalignment was postulated to have little effect on CET position [7]. This postulation seems to be supported here since the 2D model with no crystallographic orientation ability predicts CET positions reasonably well. The model's grain area predictions in the equiaxed zone are reasonably good.

A Comparison to the Hunt CET Criterion. Hunt [8] developed a method for predicting macrostructures under steady-state, Bridgman furnace conditions. According to Hunt, it is possible to produce columnar, equiaxed, or mixed structures by varying the pulling velocity and temperature gradient (V and G) in a Bridgman furnace. The Hunt model considers an observer at the columnar dendrite tips. Low temperature gradients (low G) and high growth rates (high V) at the columnar tips promote equiaxed growth. When an equiaxed volume fraction reaches 0.49, the equiaxed growth is assumed to block the columnar front and a CET is said to occur. This blocking is sometimes called 'mechanical blocking' in the literature. Hunt developed the following inequality for G to predict an equiaxed macrostructure

$$G < 0.617 D_o^{1/3} \left(1 - \left(\frac{\Delta T_N}{\Delta T_c} \right)^3 \right) \Delta T_c \quad (1)$$

where D_o is the seed density, ΔT_N is the instantaneous heterogeneous nucleation undercooling for seed particles, and ΔT_c is the undercooling at the columnar tips. Hunt also presented a diagram with V plotted against G to succinctly describe the conditions for columnar or equiaxed growth.

In this analysis, ‘mechanical blocking’ is deemed to be sufficient due to the dendritic (or non-globular) nature of the grains. For dendritic structures it is assumed the any solutal interactions occur only in the late stages of solidification and after a coherent CET structure is defined.

For a non-steady, transient situation (like in a casting), the Hunt diagram may be used to give an estimate of the CET point. In this transient case, the columnar tip velocity and the gradient at the columnar tips must be known for each time value. A locus of combined G and V at the columnar tips is superimposed onto the Hunt diagram. When the G - V locus passes into the equiaxed region of the Hunt diagram, a CET is assumed to occur. This CET prediction method is a quasi-steady approach and is reasonable because of the relatively low cooling and growth rates. Usually with enthalpy macro models of solidification, it is impossible to calculate the conditions at the columnar tips; hence, G and V are calculated for some isotherm. Typically, the liquidus isotherm is selected to get an estimate. However, a more accurate estimate is achieved by choosing an isotherm that is as close as possible to the columnar tip temperature. The liquidus isotherm velocity and the columnar tip growth rate may differ considerably, especially for low temperature gradients that change with time.

The columnar tip velocity (growth rate) was taken from one of the columnar grains of the MACE A simulation in fig. 1. Fig. 4 plots the columnar velocity versus the columnar tips position. During the columnar growth we observe local peaks and troughs in the growth rate. This behavior seems quite typical [9,10]. It is interesting to note that Gandin [9] proposed that CET occurs at a local peak in columnar growth rate when the temperature gradient is sufficiently low. On the right-hand side of the graph we see that the columnar velocity drops abruptly to zero; this signifies impingement with an equiaxed grain (that is, the CET). Just before this impingement we see some fluctuations due to thermal interactions with equiaxed grains. It would be interesting to know if a local peak in the columnar growth rate was imminent as expected from Gandin’s findings.

Fig. 4: Columnar tip velocity and undercooling versus tip position

The relationship between columnar tip velocity, V , and columnar tip undercooling, ΔT_c , is given by the equation

$$V = A \cdot \Delta T_c^n \quad (2)$$

where A is a growth constant and n is a growth index [9].

Rearranging eq. 1, the undercooling at the tip is calculated from the columnar velocity by

$$\Delta T_c = \left(\frac{V}{2.9 \times 10^{-4}} \right)^{\frac{1}{2.7}}. \quad (3)$$

Physical values for Al-Si alloys [9] are substituted into eq. 2. Fig. 4 also shows the undercooling at the columnar tips. The tip undercooling varied between 3 to 4 K. Thus, the average value of tip undercooling, ΔT_c , was taken as 3.5 K. For our analysis, we considered the 887.5 K isotherm (an undercooling of 3.5 K) as an approximation for the columnar tip position. The authors investigated this assumption and it was discovered that agreement between this isotherm and columnar tips was excellent up to the point of impingement of the columnar zone with the equiaxed zone. For reference, this isotherm is called the columnar isotherm. Fig. 5 shows the temperature gradient at the columnar isotherm versus the columnar isotherm position. The temperature gradient at the columnar isotherm started at around 30 K/cm and reduced monotonically. At the 14.3 cm position in the MACE A scenario, the columnar dendrite impinged with the equiaxed zone to give a CET. The temperature gradient at this position was approximately 7.8 K/cm. In addition, the columnar isotherm velocity at the CET position was calculated to be 0.0135 cm/s for MACE A.

Fig. 5: Temperature gradient versus the columnar isotherm position

In MACE B the CET occurred at around 13.7 cm. The temperature gradient for MACE B at the CET point was approximately 11.6 K/cm. The columnar velocity at the CET point for MACE B was calculated to be 0.0095 cm/s.

Fig. 6: Hunt map with predicted G-V locus for MACE A

The values for D_o were approximated from the experimental macrographs by grain counting and shape factor correction to be 350 cm^{-3} (0.35 mm^{-3}) for MACE A and 1600 cm^{-3} (1.6 mm^{-3}) for MACE B. In the Hunt analysis, the nucleation undercooling, ΔT_N , was estimated as 3.4 K for MACE A and 3.0 K for MACE B.

Fig. 7: Hunt map with predicted G-V locus for MACE B

Figs. 6 and 7 show the Hunt diagrams for MACE A and MACE B respectively. The columnar isotherm's G-V locus is superimposed onto each Hunt diagram. As explained earlier, where the G-V locus crosses into the equiaxed region of the chart, this is where the CET is predicted. The circular marker in these diagrams shows where the G and V values correspond to the CET.

Conclusions.

This paper presents results from a front-tracking model of the microgravity MACE experiment on CET. Fig. 1 shows good agreement between the model's prediction of CET and the experimental findings. Figs. 6 and 7 show that agreement with the Hunt map was achieved when the nucleation undercooling, ΔT_N , was estimated as 3.4 K for MACE A and 3.0 K for MACE B.

Acknowledgements

The authors wish to acknowledge the European Space Agency (ESA) for funding this research as part of CETSOL, a Microgravity Application Promotion (MAP) project. The authors also wish to acknowledge the work of EADS-Astrium for hardware development and the Swedish Space Corporation for launching the experiment.

References

- [1] Information on <http://www.ssc.se/>
- [2] Sturz L., Zimmermann G., Jung H., Mangelinck-Noël N., Nguyen Thi H., Billia B., In proceedings of the 18th ESA Symposium on European Rocket and Balloon Programmes and related research, June, 2007
- [3] L. Sturz, G. Zimmermann, *Int. J. Cast Metals Research* 20 (2007) pp122-126
- [4] S. McFadden, L. Sturz, H. Jung, N. Mangelinck-Noel, H. Nguyen-Thi, G. Zimmermann, B. Billia, D.J. Browne, D. Voss, D.J. Jarvis, *J. Jpn. Soc. Microgravity Appl.*, 25(3) (2008), pp489-494
- [5] S. McFadden and D.J. Browne., *Appl. Math. Modell.*, 33 (2009) pp 1397-1416
- [6] Zhou Y.Z., Volek A., Green N.R., *Acta Materialia*, 56 (2008) pp2631-2637
- [7] Browne D.J., *ISIJ International*, 45 (2005) pp37-44
- [8] J.D. Hunt, *Mater. Sci. Eng.*, 65 (1984) pp75-83
- [9] Ch.-A. Gandin, *Acta Mater.* 48 (2000) pp2483-2501
- [10] S. McFadden, D.J. Browne, Ch.-A Gandin, *Metall. Mater. Trans. A.*, 40A (2009) pp662-672