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Thermal characterisation with modelling for a microgravity experiment into polycrystalline equiaxed dendritic solidification with in-situ observation

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ABSTRACT

The Multiple Equiaxed Dendrite Interaction (MEDI) experiment was launched on the MASER-13 sounding rocket campaign to investigate polycrystalline equiaxed solidification in the transparent phase change material Neopentylgycol-30wt.%(d)Camphor. This material is of interest as an energy-storage material and as a transparent analogue system of solidification in hypoeutectic metal alloys with a Face Centred Cubic lattice. The liquid sample was cooled under a controlled rate of 0.75 K/min with sufficient time to allow semi-solid conditions to develop under microgravity conditions with the absence of gravity-driven convection. This manuscript provides details on the experimental apparatus and procedures. In addition, the experimental method has been augmented with a numerical model to assist with the characterisation of the essential thermal aspects of the experiment. The model followed a volume-averaging, continuum approach for mushy-zone development. A fast algorithm for computing non-isothermal crystallisation kinetics was applied to the case of binary alloy solidification. To build confidence, a formal numerical verification procedure was performed. The model converged sufficiently with second order accuracy as expected. Application of the model gave close agreement between experimental thermocouple readings and numerical simulation data with a Root Mean Square of 0.2 K for the error. A 2D thermal model is sufficient with a suitable heat loss coefficient at the sample-viewing window boundary. Thermal gradients within the sample and along the growth direction were uniform and approximately 0.3 K/mm. Lateral thermal gradients in the sample ranged from zero at the median plane to 0.3 K/mm at the boundary with the containing structure. However, temperature variation in the lateral direction was predicted to be less than 0.22 K.

1. Introduction

Under microgravity conditions, the complicating effects of gravity-driven convection and buoyancy in a liquid phase are supressed significantly. Hence, microgravity experiments are used to study solidification phenomena under diffusive conditions. Recent examples include dendritic growth in metallic alloys [1] [2] and solidification in a transparent alloy [3]. Results from microgravity experiments (and the associated modelling work) provide fundamental benchmark data that can be compared to experimental data and model outputs where gravity-driven convection is included [4] [5]. Hence, the effects of convection on the solidifying structure can be clearly understood.

The Columnar-to-Equiaxed Transition in SOLidification Processing (CETSOL) programme [6] [7] [8] is an example of a European Space Agency (ESA) Microgravity Application Promotion (MAP) that applies various microgravity platforms to study physical phenomenon. A CETSOL microgravity sounding rocket campaign, called the Multiple Equiaxed Dendrite Interaction (MEDI) experiment, was launched on December 1st, 2015 from Esrange, Sweden. The MEDI experiment was part of the MASER-13 campaign. The objectives of MEDI were to examine equiaxed dendritic nucleation, growth, interaction, and impingement in a transparent hypoeutectic alloy system, Neopentylglycol-30wt.%(d)Camphor. Observations of equiaxed dendritic solidification were made in-situ and in real-time using optical methods at macro and micro length scales.

Any microgravity experiment that is designed to investigate solidification processes for a given alloy system will benefit from the application of dedicated thermal model. However, the details of any thermal characterisation procedures—the process of applying a suitable thermal model and appropriate boundary conditions—need to be demonstrated. The risk, due to the significant challenges posed, is that boundary conditions may be assumed without detailed quantitative analysis.

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This contribution provides detail on the development and application of a numerical thermal model for the MEDI experiment and the thermal characterisation procedures used to determine appropriate boundary conditions. Thermocouple (TC) data from the experiment were compared with the model output and good agreement is demonstrated. The model provides, with confidence, a description of the thermal conditions experienced in the MEDI microgravity experiment on board the MASER-13 campaign.

1.1. Aims and objectives

The formal aims and objectives for this investigation are set out as follows:

(1) Describe the MEDI experimental set-up and procedures.
(2) Develop an appropriate thermal model of the experiment.
(3) Provide confidence in the model's numerical scheme and results.
(4) Provide an assessment of the thermal conditions experienced during the experiment.

Section 2 of this manuscript, Experimental materials and methods, expands upon the first aim. Sections 3 describes the thermal model selected for the analysis and the process of determining the boundary conditions. Section 4 provides results—both experimental and simulation results with some explanations and preliminary discussion. Section 5 provides detailed discussion on the findings of the thermal characterisation. Section 6, the conclusion section, summarises the outcomes from this manuscript in the context of the stated aims and objectives.

2. Experimental materials and methods

2.1. Neopentylglycol-(d)camphor alloy

Neopentylglycol-30wt.%(d)Camphor is a hypoeutetic alloy with a well-defined phase diagram [9]. It is of interest as an energy storage material and as an analogue to metal alloy solidification. In the liquid phase, the alloy is transparent at visible wavelengths; however, the solid phase has higher opacity to visible light. The solidifying dendritic solid can be clearly distinguished from the liquid. Significant experience had been developed with a similar alloy (with a composition of 37.5wt.%(d)Camphor) on board the TRACE microgravity campaign [3,10]. Table 1 provides thermophysical properties for the alloy. The raw materials Neopentylglycol (NPG) and (d)Camphor were purified by sublimation, alloyed under Argon atmosphere and delivered in glass syringes for filling into an evacuated experimental cell chamber.

2.2. Experiment apparatus

Airbus Defence & Space designed, built, and provided operational support on the MEDI experimental module. Fig. 1 shows the experimental cell and reference coordinate system. Fig. 2 shows a schematic for the thermal control system for the cell.

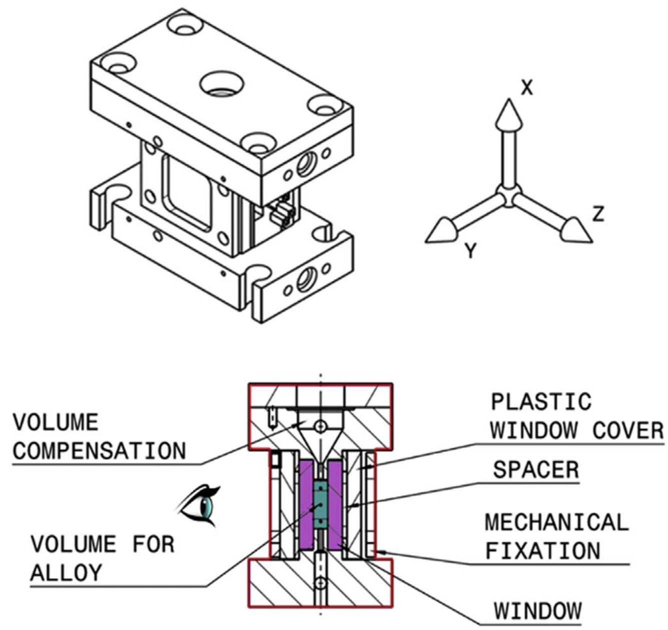

Fig. 1. MEDI experiment cell.

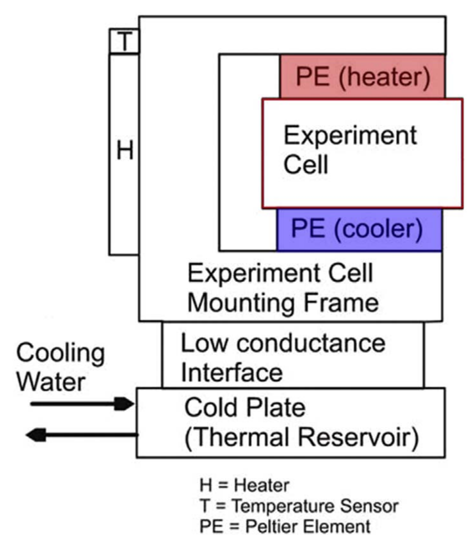

Fig. 2. MEDI experiment module.

The cell volume for containing the alloy (the central volume in Fig. 1) had nominal dimensions of 10 mm high (*H*), 13 mm wide (*W*), and 3 mm deep (*D*). A heated volume compensation reservoir was located in the top of the cell to deal with material expansion and shrinkage.

Peltier Element devices (PE in Fig. 2) were employed at the top and bottom of the cell to control the temperatures so that a temperature gradient in the *x*-direction could be established. The PE devices had thermocouples embedded within their structure to permit temperature control at each device location. However, it should be noted that these thermocouples had insufficient proximity to the boundary of the experimental cell to be considered as boundary conditions for the cell volume.

Three Ni-CrNi TCs with diameter 0.25 mm were located in the *x*-*z* median plane of the cell (see Fig. 3) and were directly in contact with the alloy material. The TCs were located at heights 1.4 mm, 4.9 mm,

Table 1
Thermophysical properties for Neopentylglycol-30%wt.-(d)Camphor.

Property	Symbol	Value	Units	Ref
Thermal conductivity of liquid	k_l	0.12	[W/mK]	[11]
Thermal conductivity of solid	k_s	0.27	[W/mK]	[11]
Density of liquid or solid	ρ	960	[kg/m^3]	
Specific heat capacity of liquid	$c_{p(l)}$	211[J/kgK] + 6.4[J/kgK^2]T		[9]
Specific heat capacity of solid	$c_{p(s)}$	940[J/kgK] + 4.2[J/kgK^2]T		[9]
Latent heat of fusion per unit mass	L	23900	[J/kg]	[9]
Equilibrium liquidus temperature	T_L	352.45	[K]	[9]
Equilibrium eutectic temperature	T_E	326.05	[K]	[9]
Melting temperature of pure NPG	T_M	404.71	[K]	[9]
Partition coefficient	k_{part}	0.072	[–]	[9]
Diffusivity of solute in liquid	D_l	97	[μm^2/s]	[9]