Fiscal Year:	FY 2018	Task Last Updated:	FY 12/29/2017
PI Name:	Beckermann, Christoph Ph.D.		
Project Title:	Effect of Convection on Columnar-to-Equiaxed Transition in Alloy Solidification		
Division Name:	Physical Sciences		
Program/Discipline:			
Program/Discipline Element/Subdiscipline:	MATERIALS SCIENCEMaterials science		
Joint Agency Name:		TechPort:	No
Human Research Program Elements:	None		
Human Research Program Risks:	None		
Space Biology Element:	None		
Space Biology Cross-Element Discipline:	None		
Space Biology Special Category:	None		
PI Email:	becker@engineering.uiowa.edu	Fax:	FY 319-335-5669
PI Organization Type:	UNIVERSITY	Phone:	319-335-5681
Organization Name:	University of Iowa		
PI Address 1:	Department of Mechanical Engineering		
PI Address 2:	2402 Seamans Center		
PI Web Page:	http://www.engineering.uiowa.edu/		
City:	Iowa City	State:	IA
Zip Code:	52242-1527	Congressional District:	2
Comments:			
Project Type:	Ground	Solicitation / Funding Source:	2010 Materials Science NNH10ZTT001N
Start Date:	03/01/2014	End Date:	02/28/2019
No. of Post Docs:	0	No. of PhD Degrees:	
No. of PhD Candidates:	3	No. of Master' Degrees:	
No. of Master's Candidates:		No. of Bachelor's Degrees:	
No. of Bachelor's Candidates:		Monitoring Center:	NASA MSFC
Contact Monitor:	Gorti, Sridhar	Contact Phone:	256 544-0158
Contact Email:	sridhar.gorti@nasa.gov		
Flight Program:			
Flight Assignment:	NOTE: End date is now 2/28/2019 per NSSC information (Ed., 12/1/15)		
Key Personnel Changes/Previous PI:			
COI Name (Institution):			
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Task Description:	ED. NOTE (7/14/2014): Project continues "Effect of Convection on Columnar-to-Equiaxed Transition in Alloy Solidification," grant #NNX10AV35G with period of performance 10/1/2010-2/28/2014. See that project for previous reporting. The project examines the mechanisms giving rise to the columnar-to-equiaxed grain structure transition (CET) during alloy solidification. On Earth, experimental investigations of the CET are affected by thermosolutal buoyant convection and grain sedimentation/flotation, making it impossible to separate these effects from the effects of solidification shrinkage and diffusive processes in determining mechanisms for the CET. Long duration microgravity experiments suppress the convective effects and grain movement, thus isolating the shrinkage and diffusive phenomena. The project increases the base of knowledge relevant to the development of solidification microstructure/grain structure of metals and alloys. Therefore, this topic is of high interest from a fundamental science point of view and it is important to those engineers practicing casting and other solidification processes. Open scientific questions include the role played by melt convection, fragmentation of dendrite arms, and the transport of fragments and equiaxed crystals in the melt. The research utilizes computational models at three different length scales: phase-field, mesoscopic, and volume-averaged models. The phase-field model is needed to resolve the growth and transport processes at the scale of the microstructure, the mesoscopic model allows for simulations of entire experiments. The models help to define and interpret previous and future microgravity and ground-based experiments.		
Rationale for HRP Directed Research:			
Research Impact/Earth Benefits:	The columnar-to-equiaxed transition (CET) in the grain structure of metal alloy castings has fascinated researchers in the solidification area for more than 50 years. The CET refers to the transition between the elongated grains in the outer portions of a casting and the more rounded grains in the center. Understanding this transition is fundamental to determining what type of grain structure forms in castings of most metal alloys (steel, aluminum, copper, etc.). Often, a fully equiaxed structure is preferred, but the fully columnar structures of many turbine blades are an important exception. In addition to its high practical significance, the CET represents a "holy grail" in the area of modeling and simulation of casting. This is because in order to realistically predict the CET, almost every physical phenomenon at every length scale must be taken into account simultaneously: heat transfer, solute transport, melt flow, and the transport of small dendrite fragments and equiaxed grains on the scale of the casting; the thermal/solutal/mechanical interactions between the growing grains/dendrites; and the nucleation of grains (especially in the presence of grain refiners) and fragmentation of existing dendrites. The research will not only provide an improved understanding of the CET, but also models and computer simulations of the grain structure formation in metal castings that can be used by industry to better understand and optimize their casting processes.		
	During the present reporting period, experiments were performed at NASA Marshall Space Flight Center using the Solidification Using a Baffle in Sealed Ampoules (SUBSA) furnace. Long, narrow cylinders of aluminum copper alloys (AlCu) were melted and then solidified in NASA's SUBSA furnace. Compositions of 4, 10, and 18 wt. % Cu were tested. The metal was contained in an alumina crucible cartridge assembly and thermocouples were attached at 9, 12, 15, and 18 cm along the crucible. The cartridge assembly was placed into the SUBSA furnace and the thermocouples tracked temperatures as the cartridge assembly was placed into the SUBSA furnace and the thermocouples tracked temperatures as the cartridge head to fully liquid near the rounded end of the crucible. At the conclusion of the holding phase, the alloys were cooled and re-solidified. Cooling rates were chosen such that CET would be present and identifiable in the solidified samples. All three samples went trough a heating phase, were held steady for a long period of time, and then were cooled and solidified. The solidified samples were removed from the crucible and then prepared for microstructure analysis by cutting, polishing, and eching. A distinct CET was only visible in the Al-18%Cu sample. The Al-10% sample showed some mixed columnar and equiaxed growth while the Al-4%Cu sample was entirely columnar. Changes will be made in order to better capture CET in future experiments, including lowering the temperature of the furnace during the holding phase of the experiment. The modelling of these experiments focused on the solidification stage, there are complications for the simulation. Simulations using the in-house OpenFOAM code will only simulate the metal cylinder itself so the question of what boundary conditions to apply are important. In order to do this, a simplified model of the SUBSA furnace was simulated using the commercial casting simulation software MAGMAsoft. If agreement can be achieved between these simulations and the experiments, time dependent		
	With good agreement in the MAGMAsoft simulation, heat fluxes can be extracted and applied in OpenFOAM. In OpenFOAM, the cylinder will be represented by an axisymmetric wedge. With the boundary conditions supplied by MAGMAsoft, the initial conditions for the solidification simulation must still be determined. It was determined that the code previously used for OpenFOAM solidification simulations was unable to handle melting. Starting the code at the steady holding phase is also not possible because it is impossible to guess or impose the distributions for the various solidification quantities in OpenFOAM. As such, the best way to initiate the simulation is to have the cylinder be entirely liquid and let the boundary conditions guide it to the steady holding phase. This should result in the proper distribution necessary for the beginning of solidification. Further work on this subject is ongoing.		
Task Progress:	The simultaneous prediction of macrosegregation and CET is still an important challenge in the field of solidification. One of the open questions is the role of melt convection in CET and the effect of CET on macrosegregation. We are developing a general multi-phase framework for modeling macrosegregation and CET. This modeling framework consists of conservation equations and constitutive relations for the two types of growth: columnar and equiaxed. The conservation equations of the model are obtained by volume-averaging the local transport equations for the solid, inter-dendritic liquid, and extra-dendritic liquid over a representative elementary volume (REV). The constitutive relation for columnar solidification are borrowed from the available relations in the literature. However, for the equiaxed solidification, the constitutive relation that are currently available in the literature are based on highly simplified assumptions and have not been validated. Therefore, instead of using these relations, we developed new accurate relations by using simulation results from a mesoscopic envelope model developed previously. In the mesoscopic		

	simulations, the evolution of the dendrite envelopes and the solute diffusion field in the extra-dendritic liquid were directly resolved on a spatial scale that corresponds to a REV. The mesoscopic results were first averaged over the REV (upscaled) and the averaged data was then used to develop accurate constitutive relations for envelope sphericity, primary tip and volume-equivalent sphere velocities, and average diffusion length. These relations were verified against the mesoscopic results and can now be used, in macroscopic models of equiaxed solidification, to incorporate more realistically the average growth kinetics and solute diffusion rates. The general multi-phase model, which accounts for undercooling both behind and in front of the columnar front, was then used to develop two different sub-models for macrosegregation during fully-columnar solidification. The first sub-model does not account for undercooling and assumes Scheil-type solidification (i.e., solidification without undercooling) behind the liquidus line. The second sub-model accounts for the primary dendrite tip undercooling and assumes Scheil-type solidification (i.e., solidification of lead 18 wt. pct. tin alloy in a side-cooled rectangular cavity. The overall macrosegregation patterns predicted by the models were found to be similar.
Bibliography Type:	Description: (Last Updated: 12/04/2024)
Articles in Other Journals or Periodicals	Neumann-Heyme H, Shevchenko N, Lei Z, Eckert K, Keplinger O, Grenzer J, Beckermann C, Eckert S. "Coarsening Evolution of Dendritic Sidearms: From Synchrotron Experiments to Quantitative Modeling." Acta Materialia, 2017 (in press), as of December 2017. , Dec-2017
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Papers from Meeting Proceedings	Neumann-Heyme H, Eckert K, Beckermann C. "Evolution of the interfacial area in dendritic solidification." 6th Decennial International Conference on Solidification Processing, Brunel University, Old Windsor, UK, July 25-28, 2017. in Proceedings of the 6th Decennial International Conference on Solidification Processing, ed. Z. Fan, BCAST, Brunel University, London, UK, 2017, p. 193-196. , Jul-2017
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