Fiscal Year:	FY 2018	**Task Last Updated:**	FY 12/29/2017
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Project Title:	Effect of Convection on Columnar-to-Equiaxed Transition in Alloy Solidification		
Division Name:	Physical Sciences		
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Program/Discipline--Element/Subdiscipline:	MATERIALS SCIENCE--Materials science		
Joint Agency Name:		**TechPort:**	No
Human Research Program Elements:	None		
Human Research Program Risks:	None		
Space Biology Element:	None		
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Space Biology Special Category:	None		
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Comments:			
Project Type:	GROUND	**Solicitation / Funding Source:**	2010 Materials Science NNH10ZTT001N
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No. of Bachelor's Candidates:		**Monitoring Center:**	NASA MSFC
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Flight Program:			
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Key Personnel Changes/Previous PI:			
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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 at the scale of individual grains, while the volume-averaged model is used to perform 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.
Task Progress:	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 heated, held at a steady temperature, and cooled. During the heating and holding portions of the experiment, the metal samples were partially melted. The fraction of alloy which was solid varied from fully solid near 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 through 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 etching. 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 phase. However, as the experiments go through a melting, a steady holding, and a solidification stage, there are complications for modeling. These complications are primarily the initial condition for simulation and the thermal boundary conditions 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 heat fluxes can be extracted from the cylinder boundary and applied in OpenFOAM. By modeling the entire furnace, properties of the various materials can be approximated and the most accurate heat fluxes can be determined. Good agreement between simulated and experimental temperatures was obtained in all cases. 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. 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 behind the primary tips. The two sub-models and the general multi-phase model were used to predict macrosegregation in a numerical solidification benchmark problem, involving columnar 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.

The model was also validated by performing macrosegregation and CET simulations of a recent benchmark solidification experiment. The overall macrosegregation map predicted by the model is similar to the macrosegregation map observed in the experiments. It consists of a region with negative lead segregation close to the bottom-right corner of the ingot and a region with positive lead segregation at the bottom-left corner. The CET positions predicted by the general model are in reasonable agreement with the CET positions observed in the experiments. Work is continuing to improve the model. Once the model is complete, it will be applied to the Al-Cu SUBSA experiments previously described in this report.

Bibliography Type:	Description: (Last Updated: 12/29/2023)
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
Articles in Peer-reviewed Journals	Zimmermann G, Sturz L, Nguyen-Thi H, Mangelinck-Noel N, Li YZ, Gandin C-A, Fleurisso, R, Guillemont G, McFadden S, Mooney R.P, Voorhees P, Roosz A, Ronafoeldi A, Beckermann, C, Karma A, Chen C-H, Warnken N, Gruen G-U, Grohn M, Poitrault I, Pehl T, Nagy I, Todt D, Minster O, Sillikens W. "Columnar and equiaxed solidification of Al-7 wt.% Si alloys in reduced gravity in the framework of the CETSOL Project." JOM Journal of The Minerals, Metals & Materials Society. 2017 Aug;69(8):1269-79. https://doi.org/10.1007/s11837-017-2397-4 , Aug-2017
Articles in Peer-reviewed Journals	Neumann-Heyme H, Eckert K, Beckermann C. "General evolution equation for the specific interface area of dendrites during alloy solidification." Acta Materialia. 2017 Nov;140:87-96. https://doi.org/10.1016/j.actamat.2017.08.021 , Nov-2017
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
Papers from Meeting Proceedings	Neumann-Heyme H, Shevchenko N, Eckert K, Grenzer J, Beckermann C, Eckert S. "Synchrotron X-ray Imaging and Numerical Modelling of Dendritic Sidebranch Evolution during Coarsening." 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. 214-217. , Jul-2017
Papers from Meeting Proceedings	Zimmermann G, Sturz L, Nguyen-Thi H, Mangelinck-Noel N, Li YZ, Liu D-R, Gandin C-A. Fleurisson R, Guillemont G, McFadden S, Mooney RP, Voorhees P, Roosz A, Ronafoeldi A, Beckermann C, Karma A, Warnken N, Saad A, Gruen G-U, Grohn M, Poitrault I, Pehl, T, Nagy I, Todt D, Minster O, Sillikens W. "Columnar and Equiaxed Solidification in a Microgravity Environment – The CETSOL Project." 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, Old Windsor, UK, July 25-28, 2017, p. 288-291. , Jul-2017
Papers from Meeting Proceedings	Torabi Rad M, Založnik M, Combeau H, Beckermann C. "Constitutive Relations for Macroscopic Modelling of Equiaxed Solidification." 6th Decennial International Conference on Solidification Processing, BCAST, 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, Old Windsor, UK, July 25-28, 2017, p. 326-329. , Jul-2017