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	FV. 2020		TV 10/05/0010
Fiscal Year:	FY 2020	Task Last Updated:	FY 12/27/2019
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		
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Zip Code:	52242-1527	Congressional District:	2
Comments:			
Project Type:	GROUND		2010 Materials Science NNH10ZTT001N
Start Date:	03/01/2014	End Date:	09/30/2021
No. of Post Docs:	0	No. of PhD Degrees:	2
No. of PhD Candidates:	1	No. of Master' Degrees:	
No. of Master's Candidates:		No. of Bachelor's Degrees:	
No. of Bachelor's Candidates:		Monitoring Center:	NASA MSFC
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Flight Program:			
Flight Assignment:	NOTE: End date changed to 9/30/2021 with new grant number awarded (80NSSC20K0828) (Ed., 9/9/20) NOTE: End date changed to 2/29/2020 per NSSC information (Ed., 2/12/19)		
	NOTE: End date is now 2/28/2019 per NSSC information	n (Ed., 12/1/15)	
Key Personnel Changes/Previous PI:			
COI Name (Institution):			
Grant/Contract No.:	80NSSC20K0828; NNX14AD69G		
Performance Goal No.:			

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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

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 **Task Description:** 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:** 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 Research Impact/Earth Benefits: 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, progress was made on performing tests to finalize the upcoming International Space Station (ISS) microgravity experiments and on modeling of the ground-based version of the experiments. Narrow cylinders of aluminum copper alloys (AlCu) were entirely melted and then solidified at Techshot Inc. using the Solidification Using a Baffle in Sealed Ampoules (SUBSA) furnace. Compositions of 4, 10, and 18 wt. % Cu were tested in two ampoule configurations. One configuration uses an alumina bottom spacer while the other uses graphite. Cooling conditions necessitate that the AlCu cylinder be 1 cm shorter for the graphite configuration. Based on temperature histories, final microstructures, and leakage behavior, the graphite configuration was chosen to for future experiments. Subsequently, a second set of AlCu cylinders was melted and solidified in the SUBSA furnace at Techshot Inc. One cylinder each of 4, 10, and 18 wt. % Cu was tested. Two cylinders of aluminum with 7 wt. % silicon (Al-7%Si) were also tested. Tests confirmed the behavior of the graphite configuration for all compositions. Preparations are now Task Progress: being made to conduct official flight and ground based experiments using the graphite configuration. Previous simulations of SUBSA cylinders in this project required unrealistic nucleation grain density values in order to predict any CET. Further improvements to the numerical code have produced CET predictions in line with experimental measurements without requiring the unrealistic values. Motion of equiaxed dendrites or fragmented dendrite arms will have a significant effect on CET prediction. To this end, a mathematical model for solidification with solid motion has been derived based on the work of Wang and Beckermann. Numerical implementation of this model is ongoing. **Bibliography Type:** Description: (Last Updated: 12/29/2023) Williams TJ, Beckermann C. "Prediction of the Columnar to Equiaxed Transition in Bottom Cooled Aluminum Copper Cylinders." Presented at TMS 2019. 148th Annual Meeting, The Minerals, Metals and Materials Society, San Antonio, Abstracts for Journals and TX, March 10-14, 2019 (invited). **Proceedings** Program. TMS 2019. 148th Annual Meeting, The Minerals, Metals and Materials Society, San Antonio, TX, March 10-14, 2019., Mar-2019 Neumann-Heyme H, Eckert K, Beckermann C. "Analysis and Modeling of Dendrite Fragmentation in Directional Solidification." Presented at Fifth International Conference on Advances in Solidification Processes (ICASP 5), Abstracts for Journals and Salzburg, Austria, June 17-21, 2019. **Proceedings** Program and abstracts. Fifth International Conference on Advances in Solidification Processes (ICASP 5), Salzburg, Austria, June 17-21, 2019. p. 85., Jun-2019 Torabi-Rad M, Beckermann C. "Simulation of Macrosegregation and Columnar to Equiaxed Transition in a Numerical Solidification Benchmark Problem." Presented at Fifth International Conference on Advances in Solidification Abstracts for Journals and Processes (ICASP 5), Salzburg, Austria, June 17-21, 2019. (invited keynote). **Proceedings** Program and abstracts. Fifth International Conference on Advances in Solidification Processes (ICASP 5), Salzburg, Austria, June 17-21, 2019. p. 3-4., Jun-2019 Torabi Rad M, Beckermann C. "A truncated-Scheil-type model for columnar solidification of binary alloys in the **Articles in Peer-reviewed Journals** presence of melt convection." Materialia. 2019 Sep;7:100364. https://doi.org/10.1016/j.mtla.2019.100364, Sep-2019