Fiscal Year:	FY 2015	**Task Last Updated:**	FY 12/26/2014
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 SCIENCE--Materials 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:	1	**No. of PhD Degrees:**	
No. of PhD Candidates:	2	**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):			
Grant/Contract No.:	NNX14AD69G		
Performance Goal No.:			
Performance Goal Text:			

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:	Progress was made in all areas of the research on the columnar-to-equiaxed transition (CET) in alloy solidification: phase-field simulation, mesoscopic simulation, and macroscopic simulation. Three-dimensional phase-field simulations of alloy solidification are being conducted to study the dendrite evolution and fragmentation process on a microscopic (microstructure) scale. Fragmented dendrite sidebranches are believed to be a potent source of equiaxed grains. For this purpose, simulations are being conducted for columnar dendritic growth with an imposed temperature gradient and cooling rate. After a fully dendritic structure is obtained, the cooling rate is suddenly reduced. This leads to fragmentation of the dendrites at the junction between primary and secondary sidebranches. The fragmentation dynamics and rates are being studied as a function of the growth conditions. Considerable effort was devoted to parallelizing the code in order to allow for large scale simulations to be conducted. During the next project year, these simulations will be continued. A theory of the evolution of the specific interface area and fragmentation is being developed. Mesoscopic simulations of columnar and equiaxed solidification are being performed in order to investigate in detail the evolution of the grain structure on an intermediate scale. In this type of simulation, the evolution of the dendrite envelopes is tracked, while the solute field is calculated only in the extra-dendritic space between the envelopes. A three-dimensional computer code has been written and simulations have been performed to compare the predicted envelope shapes with available measurements. The next step is to include melt convection. Macroscopic simulations are being conducted to study the CET on the scale of an entire casting. A volume-averaged model is used for these simulations. The governing equations are solved using the public domain OpenFoam CFD software platform. The code was tested for columnar and equiaxed solidification without melt convection and transport of solid. Gravity-driven convection and grain sedimentation/floatation have been added to the model during the past project year. Macroscopic simulations have been conducted to analyze and design future microgravity experiments.
Bibliography Type:	Description: (Last Updated: 12/29/2023)
Abstracts for Journals and Proceedings	Beckermann C. "Coarsening-Driven Dendrite Fragmentation in Directional Solidification." 4th International Conference on Advances in Solidification Processes, Old Windsor, United Kingdom, July 8-11, 2014. Conference Program. 4th International Conference on Advances in Solidification Processes, Old Windsor, United Kingdom, July 8-11, 2014. , Jul-2014
Abstracts for Journals and Proceedings	Beckermann C, Neumann-Heyme H. "Coarsening and Refinement Phenomena in Dendritic Solidification." Third International Symposium on Phase-Field Method – PFM 2014, Penn State University, State College, PA, August 26-29, 2014. Conference Program. Third International Symposium on Phase-Field Method – PFM 2014, Penn State University, State College, PA, August 26-29, 2014. , Aug-2014
Abstracts for Journals and Proceedings	Beckermann C, Neumann-Heyme H. "Concurrent Growth and Coarsening of Dendrites." Frontiers in Solidification Research, DLR, Cologne, Germany, September 2014. Conference Proceedings. Frontiers in Solidification Research, DLR, Cologne, Germany, September 2014. , Sep-2014
Articles in Peer-reviewed Journals	Yamaguchi M, Beckermann C. "Direct numerical simulation of solid deformation during dendritic solidification." JOM. 2014 Aug;66(8):1431-8. http://dx.doi.org/10.1007/s11837-014-1001-4 , Aug-2014

Awards	Neumann-Heyme H, Eckert K, Beckermann C. "Best Poster Award for 'Coarsening-Driven Dendrite Fragmentation in Directional Solidification,' 4th International Conference on Advances in Solidification Processes, Old Windsor, United Kingdom, July 8-11, 2014." Jul-2014
Papers from Meeting Proceedings	Souhar Y, De Felice VF, Založnik M, Combeau H, Beckermann C. "Three-Dimensional Mesoscopic Modeling of Equiaxed Dendritic Solidification in a Binary Alloy." 4th International Conference on Advances in Solidification Processes, Old Windsor, United Kingdom, July 8-11, 2014. 4th International Conference on Advances in Solidification Processes, Old Windsor, United Kingdom, July 8-11, 2014. Proceedings, In Press, as of December 2014. , Dec-2014