Fiscal Year:	FY 2016	**Task Last Updated:**	FY 12/30/2015
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		
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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
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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:	During the present reporting period, a Science Concept Review (SCR) was held to determine if microgravity CET experiments can be performed using the Solidification Using a Baffle in Sealed Ampoules (SUBSA) furnace on the MSL (Materials Science Laboratory). Preliminary tests at Marshall Space Flight Center indicate that the furnace is capable of melting aluminum alloys. Additional tests are to be performed in the near future to reveal if a CET can be achieved on Earth. As part of the Principal Invesitgator (PI)'s collaboration with the Columnar-to-Equiaxed Transition in SOLidification Processing (CETSOL) team in Europe, experiments were performed using a ground-based version of the Transparent Alloys instrument that is being developed by ESA (European Space Agency). The experiments use various compositions of the transparent organic alloy Neopentylglycol-(D)Camphor (NPG-DC). The present PI is responsible for the CETSOL II experiments, which are intended to simulate thermal conditions that are close to those encountered in metal casting. For this purpose, the cold and hot zones are held at all times at the same temperature, such that the adiabatic zone is close to isothermal. As opposed to the directional solidification experiments planned for CETSOL I, the sample is not moved. Instead, the cold and hot zones are cooled at a certain rate to induce solidification. The central adiabatic zone is characterized by an equiaxed dendritic grain structure. These equiaxed grains are homogeneously distributed over the experimental cell of 5 mm thickness. Experiments have been conducted to investigate the effect of the cooling rate on the nucleation and growth of the equiaxed grains. In February 2016, the PI will perform additional experiments using this setup to study different alloy compositions. The results will be used to finalize the experimental plan for the CETSOL II experiments that are being planned for the International Space Station (ISS) in 2017. Much progress has also been made during the present reporting period to develop computational models for simulating previous and future terrestrial and microgravity experiments on the CET. Models at three different length scales are investigated: 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. For simulating terrestrial experiments, the models include melt convection and transport of solid. Three-dimensional phase-field simulations of alloy solidification were conducted to study the evolution of the specific interfacial area. It is found that Sv varies in accordance with a well-known empirical equation from Speich and Fisher. This equation, which was originally developed for pure growth, fits the present data for the interfacial area density, even though dendritic solidification is characterized by concurrent growth and coarsening. The calculated temporal evolution of the inverse specific interface area is fit to a standard coarsening equation in order to determine the coarsening exponent n. Good agreement with previous studies on concurrent growth and coarsening is obtained. Additional research is necessary to obtain a generally valid relation for the evolution of the specific interface area in alloy solidification. Simulations are underway that investigate the effect of different cooling rates and other alloy characteristics on the interface evolution. Mesoscopic simulations of columnar and equiaxed solidification were 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 was written and simulations have been performed to compare the predicted envelope shapes with available measurements. During the present reporting period, these results have been carefully validated against experimental measurements. In addition, they have been used to develop constitutive equations for volume averaged models. Details are provided in the publications listed in the Bibliography section. Macroscopic simulations were conducted to study the CET on the scale of an entire casting. A volume-averaged model was used for these simulations. The governing equations were 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 is included in the model in order to simulate terrestrial experiments. During the present reporting period, much

effort was devoted to validating the model against benchmark experimental data that have been obtained by other CETSOL team members in the past. The main new feature of the present model is the inclusion of dendrite tip undercooling. Accounting for dendrite tip undercooling not only changes the solid fraction evolution, but also allows for more realistic tracking of the columnar front. A comparison of the predicted CET with the grain structure observed in the experiment shows reasonably good agreement. This agreement can be expected to improve once the movement of equiaxed grains is incorporated into the model. During the next reporting period, the macroscopic model will be used to simulate the terrestrial and microgravity experiments that are being planned for the SUBSA furnace.

Bibliography Type:	Description: (Last Updated: 12/29/2023)
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