Fiscal Year:	FY 2017	**Task Last Updated:**	FY 12/22/2016
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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
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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):			
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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 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		

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:	
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:	In March 2016, experiments were performed by the Principal Invesitgator (PI) at ACCESS in Aachen, Germany, using a ground-based version of the Transparent Alloys instrument that is being developed by the ESA (European Space Agency). The experiments used 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 experiments indicate that equiaxed dendritic dendrites indeed grow in the central adiabatic zone. These equiaxed grains are homogeneously distributed over the experimental cell of 5 mm thickness. Other experiments were conducted to investigate the effect of the cooling rate on the nucleation and growth of the equiaxed grains. The results are being used to finalize the experimental plan for the CETSOL II experiments that are being planned for the International Space Station (ISS) in 2017 or 2018. 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. A key aspect in predicting the microstructure in metal alloys is the detailed knowledge of how the shape of the solid-liquid interface evolves during solidification. Often, local features, such as the secondary dendrite arm spacing, are used for the geometrical characterization of the microstructure. However, they represent incomplete descriptions of the solid structure and their measurement can become difficult during the late stages of solidification, when the structure undergoes fundamental transformations. Alternatively, integral measures, such as the specific area of the solid-liquid interface (interface area per unit volume of solid), can be introduced to more generally characterize the overall morphology. By performing phase-field simulations for different cooling rates, we have been able to develop a general equation for the specific interface area that is valid for any cooling rate, including isothermal coarsening. This equation was validated by using data from four different synchroton tomography experiments, spanning a range of alloys and cooling rates. 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 used to develop constitutive equations for volume averaged models. For example, the sphericity of an equiaxed dendrite envelope has been related to the length of its primary arm. Also, the ratio of the solute diffusion length of the envelope to that of a sphere, which is important for calculating the internal solid fraction evolution, has been related to the envelope sphericity. These and other relations are now ready to be used in volume-averaged models of equiaxed solidification. 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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