| | | | |
|---|---|---|---|
| **Fiscal Year:** | FY 2019 | **Task Last Updated:** | FY 12/27/2018 |
| **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:** | 02/29/2020 |
| **No. of Post Docs:** | 0 | **No. of PhD Degrees:** | 1 |
| **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 changed to 2/29/2020 per NSSC information (Ed., 2/12/19)<br>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 report, progress was made on modeling of the ground-based version of the experiments to be performed on the International Space Station (ISS) and the numerical simulation of solidification of equiaxed dendrites. Very long, narrow cylinders of aluminum copper alloys (AlCu) were melted and then solidified at NASA Marshall Space Flight Center using the Solidification Using a Baffle in Sealed Ampoules (SUBSA) furnace. Compositions of 4, 10, and 18 wt. % Cu were tested. These 3 alloys represent cases in which the solid equiaxed grains will be heavier than the liquid, neutrally buoyant, and lighter than the liquid, respectively. These varying buoyancies are crucial to the modeling of the solid motion. The solidified samples were removed from the crucible and then prepared for microstructure analysis. Although the columnar-to-equiaxed transition (CET) should have been identifiable in all three alloys, it was only visible in the Al-18%Cu sample.

The modeling of the SUBSA experiments focuses on the solidification stage. 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. OpenFOAM simulations, based on the code previously developed by Torabi Rad and Beckermann, will only simulate the metal cylinder itself so the question of what boundary conditions to apply are important. In order to determine the proper initial and boundary conditions, a simplified model of the SUBSA furnace was constructed and simulated using MAGMASoft. Once agreement was achieved between these simulations and the experiments, time dependent temperature gradients were 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 temperature gradients can be determined. Agreement between simulated and experimental results was very good in all cases. After this agreement was achieved, simulations to predict the CET were conducted. Initially, these simulations neglected melt convection and solid movement. Only the Al-18%Cu case showed CET in the simulation results, and this was only achieved using unrealistic grain nucleation parameters. This confirms that considering the motion of equiaxed grains will be crucially important to more accurately predict the CET. Currently, simulations are also being conducted that consider the effect of thermal convection and solutal.

In the field of solidification, macroscale models are models that make predictions on the scale of the whole casting. These models need to incorporate phenomena that occur on the scales lower than the macroscale: microscale and mesoscale. Those phenomena can be incorporated in the macroscale models using volume-averaging methods. In these methods, which were first applied in the solidification field by Beckermann and coworkers in the 1980s and 1990s, the local equations (i.e., equations that are valid at the microscopic scale) for each phase are averaged over a volume that contains all the phases present in the system and is called the Representative Elementary Volume (REV). The volume-averaged equations contain source terms that depend on variables that are not predicted by the macroscopic model, because the lower scale information that these variables represent has been lost in the averaging process. Accurate calculation of these source terms, therefore, requires one to do a formal analysis on the REV scale and then pass up the information to the macroscale, through constitutive relations, in a process called upscaling. The term upscaling simply means that, in the ladder of length scales, information is passed up from a smaller scale to a larger scale by averaging. This upscaling has never been tried in the field of solidification, mainly because of the complexity that arises as the result of the large range of length scales that need to be resolved. In other words, in solidification, there is a large gap between the involved micro and macro length scales. Therefore, the currently available constitutive relations have been based on somewhat simplistic assumptions rather than a formal analysis of the REV scale. In this study, the gap between the micro and macro scales was bridged using the mesoscopic model of Delaleau and Beckermann. The model directly resolves the transport phenomena on the REV scale, and incorporates microscale phenomena, by using a local analytical solution for the microscale heat/solute transport. The model is used to perform three-dimensional simulations of equiaxed dendritic growth on a spatial scale that corresponds to a REV. The first set of mesoscopic simulations were performed for isothermal growth at a large range of initial undercoolings and grain densities (including a single grain).

The mesoscopic simulation results were upscaled by averaging them over the REV. For example, at any time during growth, the solute concentration field in the extra-dendritic liquid was averaged over the volume of the REV to give the average solute concentration in the extra-dendritic liquid at that time. The upscaled mesoscopic results were carefully examined and it was found that, based on the sign of the time derivative of the scaled primary arm length, the entire growth period can be divided into two stages: the variable-sphericity stage and constant-sphericity stage. The start of the constant-sphericity stage is denoted by the squares in the plot. During the variable-sphericity stage, the envelope growth is mainly due to the growth of the primary arms, while during the constant-sphericity stage, it is mainly due to the growth of the secondary arms. It was also found that using the average undercooling in the extra-dendritic liquid in the Ivantsov solution significantly underpredicts the tip velocities.

For the first time in the field of solidification, the upscaled mesoscopic results, rather than simplifying assumptions, were used to develop constitutive relations for macroscopic models of equiaxed solidification. This upscaling enabled us to present relations that incorporate changes in the shape of grains and solute diffusion conditions around them during growth. Relations were proposed for the envelope sphericity, average growth velocity, far-field undercooling that needs to be used in the Ivantsov solution to accurately predict the primary tip velocities, and for the average diffusion length around the envelopes. The constitutive relations were verified by comparing the predictions of the macroscopic model with the upscaled mesoscopic results for the isothermal cases and also for the new mesoscopic cases. These new cases involved external cooling and a recalescence in the cooling curves.

| **Bibliography Type:** | Description: (Last Updated: 12/29/2023) |
|---|---|
| **Articles in Peer-reviewed Journals** | 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. 2018 Mar;146:176-86. https://doi.org/10.1016/j.actamat.2017.12.056 , Mar-2018 |
| **Articles in Peer-reviewed Journals** | Phillion AB, Shuai S, Guo E, Wang J, Jing T, Ren Z, Neumann-Heyme H, Beckermann C, Lee PD. "Corrigendum to “Synchrotron tomographic quantification of the influence of Zn concentration on dendritic growth in Mg-Zn alloys.” (Sansan Shuai, Enyu Guo, Jiang Wang, A.B. Phillion, Tao Jing, Zhongming Ren, Peter D. Lee, Acta Materialia. 2018 Sep;156:287-96)." Acta Materialia. 2019 Feb 15;165:751-2. https://doi.org/10.1016/j.actamat.2018.11.006 [Note: reported previously in Dec 2018 as "In press, Corrected Proof; Available online 15 November 2018.'] , Feb-2019 |
| **Articles in Peer-reviewed Journals** | Torabi Rad M, Založnik M, Combeau H, Beckermann C. "Upscaling mesoscopic simulation results to develop constitutive relations for macroscopic modeling of equiaxed dendritic solidification." Materialia. 2019 Mar;5:100231. https://doi.org/10.1016/j.mtla.2019.100231 [Note: reported previously in Dec 2018 as "In Press, Accepted Manuscript. Available online 24 January 2019, 100231."] , Mar-2019 |