Fiscal Year:	FY 2018	**Task Last Updated:**	FY 12/10/2018
PI Name:	Asle Zaeem, Mohsen Ph.D.		
Project Title:	New Insights on Solid-Liquid Interface Anisotropy Effects on Solidification Patterns of Pure and Alloy Systems in Microgravity		
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:	NOTE: PI moved in summer 2018 to Colorado School of Mines from Missouri University of Science and Technology (Ed., 12/10/18)		
Project Type:	GROUND,Physical Sciences Informatics (PSI)	**Solicitation / Funding Source:**	2015-16 Physical Sciences NNH15ZTT001N-15PSI-C: Use of the NASA Physical Sciences Informatics System – Appendix C
Start Date:	02/07/2018	**End Date:**	08/30/2018
No. of Post Docs:		**No. of PhD Degrees:**	
No. of PhD Candidates:		**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:	Rogers, Jan	**Contact Phone:**	256.544.1081
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Flight Program:			
Flight Assignment:	NOTE: Grant ended early due to PI's move to Colorado School of Mines in summer 2018; end date changed to 8/30/2018 from original end date of 2/06/2020 (Ed., 8/14/19) NOTE: Period of performance and grant number changed per J. Rogers/MSFC and NSSC information (originally 1/2/18-1/1/2019 and grant number was 80NSSC18K0299)--Ed., 10/18/18		
Key Personnel Changes/Previous PI:			
COI Name (Institution):			
Grant/Contract No.:	80NSSC18K0455		
Performance Goal No.:			
Performance Goal Text:			

Task Description:	The objective of this work is to study and predict the microscale patterns that develop in solidification of pure and alloy systems in microgravity, and investigate and compare the effect of solid-liquid interface anisotropy in microgravity and terrestrial conditions. A multiscale computational framework integrating molecular dynamics simulations and phase-field modeling will be utilized to quantitatively predict solid-liquid interface properties at the nanoscale and use these data to predict solidification patterns at the microscale. Three cases will be studied to benchmark against NASA Physical Sciences Informatics (PSI) database: I. Solidification of ultra-pure succinonitrile (SCN) will be investigated; SCN is an organic crystal that forms dendrites similar to body-centered cubic (BCC) metals when it solidifies. The data generated by the Isothermal Dendritic Growth Experiment (IDGE) will be utilized to benchmark the computational modeling result for SCN. To identify similar effects in solidification patterns of BCC metals, our recent molecular dynamics (MD) simulations of iron (Fe, a BCC metal) will be utilized to build a quantitative phase-field model for predicting solidification patterns of pure Fe in microgravity. II. Solidification of pivalic acid (PVA), a face-centered cubic (FCC) organic crystal that solidifies like many non-ferrous metals, will be investigated. PVA exhibits a large anisotropy of its solid-melt interfacial energy, which is a key parameter in the selection of dendritic growth. The data generated by IDGE will be utilized to benchmark the computational modeling results for PVA. To identify similar effects in solidification patterns of FCC metals, our recent MD simulations of aluminum (Al, an FCC metal) will be utilized to build a quantitative phase-field model for predicting solidification patterns of pure Al in microgravity. III. Solidification of binary Al-Si and Al-Cu alloys will be simulated to study and compare dendritic solidification patterns in microgravity and terrestrial conditions. The data generated by MICAST/CSS (Microstructure Formation in Casting of Technical Alloys under Diffusive and Magnetically Controlled Convective. Conditions/Comparison of Structure and Segregation in Alloys Directionally Solidified in Terrestrial and Microgravity Environments) 6 & 7 on Al-Si will be utilized to validate the computational modeling results. The recently developed phase-field finite-element models in Principal Investigator's (PI) research group for predicting dendritic solidification patterns in pure and alloy systems will be modified and implemented in the Idaho National Lab's MOOSE framework (Multiphysics Object-Oriented Simulation Environment) to study and predict three-dimensional microstructures of solidification. The required nanoscale input parameters for phase-field models, such as interface energies and anisotropy of SCN, PVA, Al-Si, and Al-Cu will be calculated by MD simulations. It is essential to notice that most of the current mesoscale computational models do not include the actual interface energies and anisotropy coefficients, and only utilize arbitrary values to generate the desired patterns. The main focus of this work will be on studying the effects of solid-liquid interface properties on solidification patterns in microgravity condition; moreover some simulations at terrestrial gravity will be completed to compare the patterns at microgravity and terrestrial conditions. The validation in microgravity condition is particularly essential in order to confidently use the proposed multiscale model to study other pure and alloy materials in microgravity condition and compare their microstructures and segregation regions to those in terrestrial gravity. The multiscale computational models that will be developed in this work can be used later to study solidification microstructures of other pure and binary alloys, and can be extended to study ternary alloys and ferrous metals in microgravity; this will result in developing the capability of accurately predicting solidification patterns and microstructures that develop in casting, welding, and laser and/or electron beam additive manufacturing in microgravity. Editor's note August 2019: Grant ended early due to PI's move from Missouri University of Science and Technology to Colorado School of Mines in summer 2018 ; original period of performance for this grant was 2/7/2018-2/06/2020. Project continues as "New Insights on Solid-Liquid Interface Anisotropy Effects on Solidification Patterns of Pure and Alloy Systems in Microgravity," grant 80NSSC19K0569.
Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	The surface and interface forces become dominant in the absence of the Earth's gravity, which make it possible to fundamentally study their effects on solidification patterns and microstructures. The proposed multiscale computational model that is being developed in this work is a predicative tool to study solidification microstructures of other pure and binary alloys, and it can be extended to study ternary alloys and ferrous metals. The outcome of this project is helpful in predicting nano and microstructures that develop in casting, welding, and laser and/or electron beam additive manufacturing, and consequently enables prediction of property and performance of such products.
Task Progress:	This project is completely a computational modeling and simulation project in which the experimental data from previous NASA experiments will be utilized to verify and validate the models. The Principal Investigator (PI) is an expert in molecular dynamics simulations and phase-field modeling to ensure completing the proposed computational tasks, and he has already established his Computational Materials and Mechanics Laboratory in the Colorado School of Mines (CSM). The first version of the phase-field modeling framework is created in order to study the solid-liquid interface anisotropy effects on solidification patterns of pure systems. First, the solidification of ultra-pure succinonitrile (SCN) is being investigated; the data generated by the Isothermal Dendritic Growth Experiment (IDGE) will be utilized to benchmark the computational modeling result for SCN. To identify similar effects in solidification patterns of BCC metals, our recent molecular dynamics (MD) simulations of iron (Fe, a BCC metal) is being utilized to build a quantitative phase-field model for predicting solidification patterns of pure Fe in microgravity. After validation and verification of this framework, it will be extended first to FCC pure metals and then to alloy systems. The NASA experimental data on pivalic acid (PVA), a face-centered cubic (FCC) organic crystal, will be utilized to validate the framework for FCC pure system and then solidification of binary Al-Si and Al-Cu alloys will be simulated to study and compare dendritic solidification patterns in microgravity and terrestrial conditions. The data generated by MICAST/CSS 6 & 7 on Al-Si will be utilized to validate the computational modeling results. The goal is to quantitatively predict solid-liquid interface properties at the nanoscale and use these data to predict solidification patterns at the microscale. Editor's note August 2019: Grant ended early due to PI's move from Missouri University of Science and Technology to Colorado School of Mines in summer 2018 ; original period of performance for this grant was 2/7/2018-2/06/2020. Project continues as "New Insights on Solid-Liquid Interface Anisotropy Effects on Solidification Patterns of Pure and Alloy Systems in Microgravity," grant 80NSSC19K0569. See that project for subsequent reporting.

Bibliography Type:	Description: (Last Updated: 03/23/2022)