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 Microgravity	e Anisotropy Effects on Soli	diffication Patterns of Pure and Alloy Systems in
Division Name:	Physical Sciences		
Program/Discipline:			
Program/Discipline Element/Subdiscipline:	MATERIALS SCIENCEMaterials sc	cience	
Joint Agency Name:	Т	echPort:	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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City:	Golden	State:	СО
Zip Code:	80401	<b>Congressional District:</b>	7
Comments:	NOTE: PI moved in summer 2018 to C (Ed., 12/10/18)	Colorado School of Mines fr	om Missouri University of Science and Technology
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:	I	No. of Bachelor's Degrees:	
No. of Bachelor's Candidates:		Monitoring Center:	NASA MSFC
Contact Monitor:	Rogers, Jan	<b>Contact Phone:</b>	256.544.1081
Contact Email:	jan.r.rogers@nasa.gov		
Flight Program:			
Flight Assignment:	NOTE: Grant ended early due to PI's n 8/30/2018 from original end date of 2/0 NOTE: Period of performance and gran 1/2/18-1/1/2019 and grant number was	nove to Colorado School of 06/2020 (Ed., 8/14/19) nt number changed per J. Re 80NSSC18K0299)Ed., 10	Mines in summer 2018; end date changed to ogers/MSFC and NSSC information (originally 0/18/18
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: 1. Solidification of ultra-pure succinonitrile (SCN) will be investigated; SCN is an organic crystal that forms dendrites in solidification patterns of BCC metals, our recent molecular dynamics (MD) simulations of iron (Fe, a BCC metal) 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) simulatical 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 corgarity Evironments) 6 & 7 on Al-Si will be utilized to validate the computational modeling results. The recently developed phase-field finite-element models in Principal Investigate's (PI) research group for predicting dendritic solidification patterns of pure Al in microgravity und the result and will be
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 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 An

**Bibliography Type:** 

Description: (Last Updated: 06/13/2025)