Fiscal Year:	FY 2020	**Task Last Updated:**	FY 02/20/2020
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		
PI Email:	zaeem@mines.edu	**Fax:**	FY
PI Organization Type:	UNIVERSITY	**Phone:**	(303) 384-2260
Organization Name:	Colorado School of Mines		
PI Address 1:	Department of Mechanical Engineering & Materials Science Program		
PI Address 2:	1523 Illinois St., CoorsTek 203		
PI Web Page:			
City:	Golden	**State:**	CO
Zip Code:	80401	**Congressional District:**	7
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:	04/25/2019	**End Date:**	04/21/2021
No. of Post Docs:		**No. of PhD Degrees:**	
No. of PhD Candidates:	1	**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:	Su, Ching-Hua	**Contact Phone:**	256-544-7776
Contact Email:	ching.h.su@nasa.gov		
Flight Program:			
Flight Assignment:	NOTE: End date changed to 4/21/2021 per NSSC information (Ed., 9/9/20) NOTE: Period of performance per C-H Su/MSFC is 4/25/2019-4/20/2020 (Ed., 8/14/2019)		
Key Personnel Changes/Previous PI:			
COI Name (Institution):			
Grant/Contract No.:	80NSSC19K0569		
Performance Goal No.:			
Performance Goal Text:			

Task Description:	NOTE: Continuation of "New Insights on Solid-Liquid Interface Anisotropy Effects on Solidification Patterns of Pure and Alloy Systems in Microgravity," grant 80NSSC18K045, when Principal Investigator was affiliated with Missouri University of Science and Technology. 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.
Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	Since solid-liquid interfacial forces become dominant in the absence of the Earth's gravity, we hypothesize that the proposed solidification phase field-simulations in microgravity conditions will enable us to fundamentally understand and distinguish transport phenomena, defect formation, and microstructural evolution mechanisms in traditional and advanced (e.g., additive) manufacturing processes in Earth's gravity.
Task Progress:	1. A multicomponent multiphase-field model for solidification of alloys systems under microgravity condition is developed. 2. A comprehensive study is completed by simulating solidification of Al-Cu system under microgravity condition to investigate the effect of solid/liquid interfacial energy anisotropy on: - Primary Dendrite Arm Spacing ; - Primary Dendrite Trunk Diameter ; - Secondary Dendrite Arm Spacing ; - Primary Dendrite Average Growth Rate ;- Theta-phase (Al_2Cu) fraction
Bibliography Type:	Description: (Last Updated: 03/23/2022)