Fiscal Year:	FY 2022	**Task Last Updated:**	FY 03/21/2022
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:**	09/24/2021
No. of Post Docs:	1	**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 9/24/2021 per NSSC information (Ed., 4/22/21) 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:	A PhD student and postdoc are partially supported to determine the solid-liquid interface energies and their anisotropy for Ti and Al-Cu alloys by molecular dynamics simulations		
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.

Solidification of pure Al and Ti, and binary Al-Cu alloys are 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 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 Al-Cu alloys are 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:

The objective of this project was to study the effects of solid-liquid (SL) interfacial energy and its anisotropy on the microstructure development during the solidification of pure and binary systems. For this purpose, we developed an atomistic-informed phase-field (PF) framework to study the solidification of pure metals and binary materials. The simulations were run in microgravity conditions. Molecular dynamics (MD) was used to determine the anisotropic kinetic coefficient, SL interface energy, and other material properties to parameterize the PF models and the PF model predicts the formation and evolution of SL interface that affects the microstructures and properties of solidified metals and alloys. As a benchmark example for the solidification of alloys, we investigated the interactive effects of Cu concentration, SL interfacial energy properties, and cooling conditions on dendrite pattern and dendrite growth mechanisms during the solidification of Al-Cu alloys. In addition, we have developed a new atomistic-informed PF model for investigating the rapid solidification of pure materials. Unlike previous models and to consider the actual physics of crystal growth, the PF parameters, representing interface mobility, SL transformation barrier, and interfacial energy gradient, are temperature dependent. The parameters are determined by a combination of MD simulations and classical thermodynamic calculations based on the temperature-dependent SL interface properties and kinetic coefficient. For the benchmark example of Ti, the MD results show the average SL interface energy decreases with temperature, and the preferred dendrite growth direction shifts from <100> to <110> direction as the undercooling increases. PF simulations also show other favorite growth directions, implying that there is a competition between the interface anisotropy and kinetics of the SL interface. We specially investigated solidification of four Al-Cu alloys with 3%, 6%, 8.4%, and 10.6 at% Cu using atomistic-informed multi-phase field modeling. We investigated the combined effects of cooling condition, alloy composition and interfacial energy anisotropy on second phase (theta-phase) fraction and its distribution, and growth dynamics and morphology of solidification structures. First, the CM interfacial energies and its anisotropy were determined using molecular dynamic simulations. These values were used in phase-field simulations to quantitatively investigate the interactive effects of Cu content, CM interfacial properties, and cooling condition on growth dynamics and solidification patterns. Specific findings include the following: 1- Molecular dynamics simulation results showed that the CM interfacial energy decreases linearly with increasing Cu content while its anisotropy does not show a specific trend. 2- Phase-field simulation results showed that with increasing the cooling rate, the dendrite arm spacing and the amount of theta-phase decrease, and this reduction is more pronounced in alloys with higher Cu content. Also, the theta-phase fraction decreases by increasing the heat transfer coefficient. This reduction is due to the higher undercooling needed for eutectic reaction, which results in the formation of higher alpha-phase, and less liquid transforms into alpha+theta phase via eutectic reaction. Furthermore, the coring phenomenon is more noticeable at higher cooling rates which results in a reduction in Cu content in the interdendritic regions and a decrease in theta-phase. 3- Distribution of theta-phase is more homogenous in alloys with seaweed structures (Al-3 and Al-8.4 at% Cu) than the alloys with dendritic structures. In all investigated alloys, the distribution of theta-phase becomes more homogenous by increasing the heat transfer coefficient, but it is more sensitive to the value of heat transfer coefficient with seaweed structures. 4- Anisotropy of CM interfacial energy has a significant effect on solidification patterns and their growth dynamic. At the limit of diffusion control growth, when the strength of anisotropy is higher than 0.005 dendritic morphology is dominant at all cooling rates. At lower CM interfacial energy anisotropy different seaweed structures can form regarding constitutional supercooling at ahead of growing tip. When supercooling is less than 8K degenerate or fractal seaweed form while at higher supercoolings compact seaweed is dominant microstructure.

	The results of this research are published in S. Kavousi, A. Gates, L. Jin, M. Asle Zaeem. A temperature-dependent atomistic-informed phase-field model to study dendritic growth, Journal of Crystal Growth 579 (2022), 126461 G. Azizi, S. Kavousi, M. Asle Zaeem, Interactive Effects of Interfacial Energy Anisotropy and Solute Transport on Microstructure Evolution of Al-Cu Alloys during Solidification Accepted in Acta Materialia (2022).
Bibliography Type:	Description: (Last Updated: 03/23/2022)
Articles in Peer-reviewed Journals	Kavousi S, Gates A, Jin L, Asle Zaeem M. "A temperature-dependent atomistic-informed phase-field model to study dendritic growth." Journal of Crystal Growth. 2022 Feb 1;579:126461. https://doi.org/10.1016/j.jcrysgro.2021.126461 , Feb-2022
Articles in Peer-reviewed Journals	Azizi G, Kavousi S, Asle Zaeem M. "Interactive effects of interfacial energy anisotropy and solute transport on solidification patterns of Al-Cu alloys." Acta Materialia. 2022 Mar 22. https://doi.org/10.1016/j.actamat.2022.117859 , Mar-2022