Fiscal Year:	FY 2020	**Task Last Updated:**	FY 05/29/2020
PI Name:	Ankit, Kumar Ph.D.		
Project Title:	Advanced Modeling and Simulation of Crystal Growth Dynamics		
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:	kumar.ankit@asu.edu	**Fax:**	FY
PI Organization Type:	UNIVERSITY	**Phone:**	480-965-4541
Organization Name:	Arizona State University		
PI Address 1:	School for Engineering of Matter, Transport and Energy		
PI Address 2:	551 E Tyler Mall, ERC 265		
PI Web Page:			
City:	Tempe	**State:**	AZ
Zip Code:	85287	**Congressional District:**	9
Comments:			
Project Type:	GROUND	**Solicitation:**	2017 Physical Sciences NNH17ZTT001N--17PSI-D: Use of the NASA Physical Sciences Informatics System – Appendix D
Start Date:	08/01/2018	**End Date:**	07/31/2020
No. of Post Docs:	0	**No. of PhD Degrees:**	0
No. of PhD Candidates:	1	**No. of Master' Degrees:**	0
No. of Master's Candidates:	0	**No. of Bachelor's Degrees:**	0
No. of Bachelor's Candidates:	0	**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 7/31/2020 per NSSC information (Ed., 5/4/2020)		
Key Personnel Changes/Previous PI:	May 2020 report: The co-Investigator listed on this project, Dr. Martin Glicksman, will be retiring this summer from the Florida Institute of Technology (FIT).		
COI Name (Institution):	Glicksman, Martin Ph.D. (Florida Institute of Technology)		
Grant/Contract No.:	80NSSC18K1440		
Performance Goal No.:			
Performance Goal Text:			

Task Description:	Recent theoretical analyses of the Isothermal Dendritic Growth Experiment (IDGE) archived in the NASA Physical Sciences Informatics (PSI) system reveals the presence of a fourth-order interfacial scalar field, termed the bias field, that works in the background and dynamically couples with interface normal motion. Solid-liquid interfaces support such scalar perturbation fields by adding or withdrawing small amounts of thermal energy. Preliminary insights suggest that perturbation fields modulate interface motion and can stimulate pattern formation depending upon the interface's curvature distribution. However, our current understanding of the factors that govern the intensity of capillary-mediated fields is limited to pure melts and to two spatial dimensions. Moreover, any quantitative understanding of the intensity threshold beyond which such capillary-mediated fields can potentially modulate pattern formation is all together, absent. The goal of the PSI project is to explore this fascinating autogenous mechanism of pattern formation by leveraging the IDGE data. Surface curvature and crystal-melt anisotropy strongly influence bias fields. Motivated by our recent detection of perturbation fields on grain boundary grooves (GBGs), which also appear to explain the anomaly reported in the microgravity data, the underlying hypotheses which we intend to test are: (a) weak capillary fields that are resident on solid-liquid interfaces modulate the shapes of melting crystalline fragments, and (b) shape perturbations from capillary fields amplify on unstable interfaces, and instigate instabilities on interfacial regions of equilibrated GBGs. Our 3D phase-field simulations on grooving will provide unprecedented insights into this fascinating autogenous mechanism of pattern formation and might also enable us to develop novel processing methods to improve microstructure-level control in alloy castings. The associated issue of comparing the efficacy of noise amplitude to the bias field intensity--fundamental issue in understanding pattern formation--will also be investigated theoretically and via the phase-field techniques.
Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	The physical interface mechanism explored in this study shows that capillary-mediated fields provide perturbations capable of initiating diffusion-limited patterns. These include patterns in nature exhibited by snowflakes and crystallized mineral forms, as well as microstructures of cast alloys. Capillary-mediated interface fields might provide new approaches toward achieving improvements in solidification processing, welding, and crystal growth by control of microstructure at mesoscopic scales.
Task Progress:	- The synergy between the phase-field simulations and theoretical findings validate the unique presence of bias-fields on isolated grain boundary groove surfaces. - Analysis of periodic grain boundary grooves was performed, which is a critical step for generalizing the idea of bias-fields. These findings will be compared with phase-field simulations to validate the underlying hypotheses. - It is discovered that melt convection can induce growth competition in seaweed-like solidifying microstructures that have nearly isotropic or weakly-anisotropic surface energies.
Bibliography Type:	Description: (Last Updated: 06/10/2020)
Articles in Peer-reviewed Journals	Ankit K, Glicksman M. "Growth competition during columnar solidification of seaweed microstructures." Eur Phys J E Soft Matter. 2020 Feb 25;43(2):14. https:// ; PMID: 32086596 , Feb-2020
Articles in Peer-reviewed Journals	Glicksman M, Ankit K. "Thermodynamic behaviour of solid–liquid grain boundary grooves." Philosophical Magazine 2020. Published Online: 14 Mar 2020. https:// , Mar-2020
Articles in Peer-reviewed Journals	Laxmipathy V, Wang F, Selzer M, Nestler B, Ankit K. "Influence of melt convection on the morphological evolution of seaweed structures: Insights from phase-field simulations." Computational Materials Science. 2019 Dec;170:109196. https:// , Dec-2019
Journal/Magazine covers	Ankit K, Glicksman M. "Cover in the journal The European Physical Journal E for the article, 'Growth competition during columnar solidification of seaweed microstructures.' " The European Physical Journal E. 2020 February;43(2):14. , Feb-2020