Fiscal Year:	FY 2019	**Task Last Updated:**	FY 05/31/2019
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		
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Comments:			
Project Type:	GROUND,Physical Sciences Informatics (PSI)	**Solicitation / Funding Source:**	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
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Flight Program:			
Flight Assignment:	NOTE: End date changed to 7/31/2020 per NSSC information (Ed., 5/4/2020)		
Key Personnel Changes/Previous PI:			
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:	To understand the origin of natural patterns, and, ultimately, control microstructures derived from materials processes involving solidification, welding, and crystal growth, one must determine: (1) whether pattern-forming ‘‘signals’’ or ‘‘instructions’’ exist, and, if so, (2) do they fundamentally devolve from stochastic processes, or from higher-order deterministic sources. Our research addresses both issues for crystal-melt interfaces in unary systems, by exploring the presence of interfacial energy fields that provide pattern-forming stimuli in 2D. We detected and measured the presence of such stimuli on solid-liquid interfaces through novel measurements extracted from phase-field simulations. Capillary fields in the form of interfacial energy distributions are exposed and measured on simulated microstructures in the form of equilibrated solid-liquid grain boundary grooves (GBGs). Simulated interfacial data also allow quantifiable comparison with analytic predictions of interfacial energy fields derived from sharp-interface thermodynamics. Simulations and measurements that we report also confirm that equivalent pattern-forming fields arise within standard phase-field physics that manifest themselves as deterministic perturbations. Numerical simulations are compared with predictions based on interface energy conservation and classical field theory. The comparison reveals the existence of persistent capillary-mediated energy fields that influence the dynamics of interfacial shape changes during phase transformation. Such fields stimulate complex pattern formation on unstable interfaces with, or without, the benefit of noise. As melt convection can interact with capillary-mediated bias-fields, a Navier-Stokes coupled phase-field solver was also developed to analyze the influence of this interaction on the evolution of directionally-solidified patterns. To verify our findings, in future, we will compare the morphological evolution as predicted by the bias-field theory and the phase-field simulations during dendritic growth and shrinkage with the IDGE (Isothermal Dendritic Growth Experiment) data that is currently archived in the NASA-PSI.
Bibliography Type:	Description: (Last Updated: 11/17/2022)
Abstracts for Journals and Proceedings	Glicksman ME, Ankit K. "Melting in Microgravity: How crystallite shape changes led to new insights about interface dynamics." Presented at the 7th International Conference on Solidification and Gravity (SG 18), Miskolc-Lillafüred, Hungary, September 3-6, 2018. Proceedings of Solidification and Gravity 2018 Sept. p. 41. , Sep-2018
Abstracts for Journals and Proceedings	Glicksman ME, Ankit K. "Detection of Capillary-Mediated Interface Energy Fields Using Phase-Field Residuals." Presented at the SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS 18), Portland, OR, July 9-13, 2018. SIAM MS 18 conference, July 9-13, 2018. p. 261. , Jul-2018
Abstracts for Journals and Proceedings	Glicksman ME, Ankit K. "Capillary-Mediated Solid-Liquid Energy Fields: Their detection using grain boundary grooves and phase-field method." Presented at the 5th International Conference on Advances in Solidification Processes (ICASP-5) 5th International Symposium on Cutting Edge of Computer Simulation of Solidification, Casting and Refining (CSSCR-5), Salzburg, Austria, June 17-21, 2019. ICASP-5 CSSCR-5 2019 Conference, June 2019. Abs ID: 5. , Jun-2019
Abstracts for Journals and Proceedings	Glicksman ME, Ankit K. "Capillary-mediated interface fields." Presented at the 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19), Keystone, CO, July 28-August 2, 2019. 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19), Keystone, CO, July 28-August 2, 2019. Information at https://www.iccge19.org , Jul-2019

Articles in Peer-reviewed Journals	Glicksman ME, Ankit K. "Capillary-mediated solid-liquid energy fields: their detection with phase-field method." IOP Conference Series: Materials Science and Engineering. 2019 May;529(1):012027. https://doi.org/10.1088/1757-899X/529/1/012027 , May-2019
Awards	Glicksman ME, Ankit K. "2018 Robert W. Cahn Prize awarded by Springer Nature and the Journal of Materials Science, August 2018. See https://www.springer.com/gp/materials/cahn-prize-2018 " Aug-2018