

Fiscal Year:	FY 2022	Task Last Updated:	FY 11/14/2022
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 NNN17ZTT001N-17PSI-D: Use of the NASA Physical Sciences Informatics System – Appendix D
Start Date:	08/01/2018	End Date:	07/31/2022
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
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Flight Program:			
Flight Assignment:	NOTE: End date changed to 7/31/2022 per NSSC information (Ed., 11/8/21) NOTE: End date changed to 7/31/2021 per NSSC information (Ed., 9/9/2020) NOTE: End date changed to 7/31/2020 per NSSC information (Ed., 5/4/2020)		
Key Personnel Changes/Previous PI:	None		
COI Name (Institution):	Glicksman, Martin Ph.D. (Florida Institute of Technology)		
Grant/Contract No.:	80NSSC18K1440		
Performance Goal No.:			
Performance Goal Text:			

Task Description:	<p>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.</p> <p>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.</p>
Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	<p>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.</p>
Task Progress:	<p>In this project, we comparatively analyzed capillary-mediated fields up to fourth-order, including the surface Laplacian of a profile's chemical potential. This Laplacian is proportional to scaled divergences of fluxes that appear on counterpart real or simulated microstructures with congruent shapes. Divergent energy fluxes manifest as cooling distributions, which cause depression of the thermochemical potential measured along diffuse interfaces simulated with the phase-field technique. Cooling distributions were visualized to explain qualitative and quantitative features of a microstructure's steady-state thermal maps. The findings of this project provide evidence of how the thickness and shape of crystal-melt interfaces co-determine whether, and to what extent, interfacial transport occurs. Understanding the origin and actions of interfacial capillary fields might offer improved control of microstructure at mesoscopic levels, accessible with these deterministic fields through physical and chemical means.</p>
Bibliography Type:	Description: (Last Updated: 11/17/2022)
Articles in Peer-reviewed Journals	<p>Glicksman M, Wu P, Ankit K. "Periodic grain boundary grooves: Analytic model, formation energies, and phase-field comparison." J. Phase Equilib. Diffus. 2022 July 22. https://doi.org/10.1007/s11669-022-00967-4 , Jul-2022</p>
Articles in Peer-reviewed Journals	<p>Glicksman M, Ankit K, Wu P. "Capillary effects on curved solid-liquid interfaces: An overview." Journal of Crystal Growth. 2022 Sept 15. https://doi.org/10.1016/j.jcrysgro.2022.126871 , Sep-2022</p>