Fiscal Year:	FY 2018	**Task Last Updated:**	FY 09/05/2018
PI Name:	Eshraghi, Mohsen Ph.D.		
Project Title:	Pore-Mushy Zone Interaction during Directional Solidification of Alloys: Three Dimensional Simulation and Comparison with Experiments		
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:**	2015 Physical Sciences NNH15ZTT001N-15PSI-B: Use of the NASA Physical Sciences Informatics System – Appendix B
Start Date:	09/16/2016	**End Date:**	09/15/2019
No. of Post Docs:		**No. of PhD Degrees:**	
No. of PhD Candidates:	2	**No. of Master' Degrees:**	1
No. of Master's Candidates:	2	**No. of Bachelor's Degrees:**	2
No. of Bachelor's Candidates:	2	**Monitoring Center:**	NASA MSFC
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Flight Program:			
Flight Assignment:	NOTE: Extended to 9/15/2019 per NSSC information (Ed., 9/12/18)		
Key Personnel Changes/Previous PI:			
COI Name (Institution):	Tewari, Surendra Ph.D. (Cleveland State University) Felicelli, Sergio Ph.D. (University of Akron)		
Grant/Contract No.:	NNX16AT75G		
Performance Goal No.:			
Performance Goal Text:			

Task Description:	Formation of shrinkage porosity and bubbles during solidification disturbs the dendritic array network and seriously degrades the mechanical properties of castings, whether these are large commercial castings of aluminum or steel alloys or a small directionally solidification single crystal turbine blade. Since in-situ observation of the interaction of pores/bubbles with the primary dendrite array in the mushy zone is not feasible in opaque metal alloys, transparent organic alloys solidifying in narrow gapped rectangular cross-section glass crucibles have been extensively used for such studies. However, all these observations are essentially between bubble and a two-dimensional (2D) array of primary dendrites and are affected by the wall effects. Analytical and numerical modeling of pore formation and migration in mushy zone have also been 2D. Contrary to earlier belief, it is now recognized that the basic premise of such experiments, i.e., 2D dendrites represent morphology of a three-dimensional (3D) array, is false. Understanding pore-mushy zone interaction in real castings requires both the experimental observations and also the theoretical/numerical modeling with 3D array of dendrites. Pore Formation and Mobility Investigation (PFMI) experiments were conducted in the microgravity environment aboard the Space Station with the intent of better understanding the role entrained porosity/bubbles play on microstructure during controlled directional solidification (DS). Although, the PFMI investigators have qualitatively described some of their observed interactions between the pore and mushy zone, no attempt has been made to analytically or numerically model these observed mushy zone disturbances caused by the presence of bubbles during directional solidification. Purpose of this research is to develop a numerical 3D model which can simulate the pore-mushy zone interaction during directional solidification of Succinonitrile-Water alloys in microgravity and test the simulation results against the PFMI microstructural observations, quantitatively and qualitatively. Several sets of time-temperature-interface-bubble interaction data will be extracted and analyzed from the PFMI videos for this purpose. In order to achieve this goal, we will exploit forefront methods in microscale solidification. We propose a methodology based on cellular automaton (CA) to track the interface and Lattice Boltzmann (LB) to solve the transport equations and simulate pore formation and its motion during directional solidification. The outcome of the proposed research will be an unprecedented tool to numerically simulate the pore-mushy zone interaction during directional solidification in a 3D domain, providing critical information on microstructure response to process parameters. This will have a huge impact on the design of improved mushy zone models based on the microstructure information obtained from the direct simulation. The developed knowledge will advance the state of understanding of solidification phenomena in the microscale, will contribute to improved numerical predictions of porosity formation, and will advance the state of the art in LB methods for simulating transport phenomena. PFMI is the only 3D spatial/temporal observation of pore-mushy zone interactions available to make qualitative/quantitative comparisons with our 3D LB-CA results as a unique model for large scale simulations of pore-mushy zone interactions with a micro-scale resolution.
Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	This investigation will help explain fundamental aspects of the mechanisms that regulate the formation of microporosities. The formation of these defects depends on microstructure features that cannot be properly captured by current meso- and macro-scale models based on averaging techniques. The direct numerical simulation of bubble dynamics in a dendritic network will provide a relation between macroscopically observable variables like cooling rate or temperature gradient and difficult to measure dynamic microscopic features like microporosity distribution, interdendritic permeability, solute redistribution, and dendrite arm spacing. It is expected that this research will not only provide valuable contribution to the understanding of pore-mushy zone interaction during solidification in the absence of gravity, which would be helpful for future in-space fabrication processes involving solidification, but it will be a crucial first step to quantitatively simulate such 3D interactions during terrestrial directional solidification in realistic size sample domains. Although much observation has been done in pictures of static microstructures at different stages of solidification, it has never been possible to capture the dynamic response of these features in an evolving mushy zone. This information is critical to assess, validate, and improve macroscale mushy zone models used in current casting and welding codes.
Task Progress:	Due to the temperature difference at the interface of the bubble and surrounding fluid, Marangoni convection causes fluid flow during solidification. Most of previous works on simulation of bubble-dendrite interactions ignore the Marangoni effect while it can have a significant effect especially in microgravity conditions where natural convection is absent. The Pore Formation and Mobility Investigation (PFMI) experiments at International Space Station (ISS) have shown that pores and bubbles adhered to the ampoule walls can change the morphology of dendrites and affect the growth kinetics. We used our numerical models to simulate the Marangoni effect and bubble-dendrite interactions during solidification of binary alloys. Effect of Marangoni convection on dendrite growth and bubble-dendrite interactions under microgravity and terrestrial conditions were studied. A Phase Filed (PF)-Lattice Boltzmann (LB) model was developed to simulate in bubble-dendrite interactions. Using the developed model, interaction of growing dendrites with a big bubble attached to a wall was simulated. The bubble diameter was about two times as big as the primary dendrite arm spacing, similar to what is observed in PFMI-15 experiment. The simulation considered Marangoni convection in the absence of gravity. The results showed that the dendrite branch in vicinity of the bubble grow slower compared to the dendrites far from the bubble. Also side branching is enhanced in the vicinity of the bubble. Two dimensional (2D) models are usually unable to capture all features of microstructures that are determinative in many materials properties, especially when fluid flow is involved. It is known that melt flow can significantly alter the growth kinetics by affecting solutal gradient around the dendrites, and moving the bubbles. While melt convection is blocked by dendrite arms in 2D simulations, flow can go around the 3D arms which results in a different bubble distribution and dendritic morphology. Studies have shown that the growth of dendrites in 3D is considerably different from 2D. Therefore, in order to obtain correct physical results, it is necessary to perform the simulations in 3D. The thermocapillary flow field associated with a bubble in PFMI-15 experiment was investigated. The flow path was tracked by following miniature detached dendrite branches that made circular routes from the interface, through the bulk liquid, and back, and showed that a flow field which extended 4.5 mm into the melt had average velocity of ~0.1 mm/s and another one that extended 2.5 mm averaged ~0.4 mm/s. We followed similar tracer dendrite branches as they enter from the melt into the mushy-zone and after traversing certain distance in the mush come back out into the melt. This observation showed that the flow speed in the mushy region is higher than that in the bulk melt, which was puzzling and was considered for our numerical simulations. Another interesting observation from the PFMI videos was that the tracer dendrite branches invariably accelerated as they approached the solid/liquid (S/L) interface.

We performed large-scale three-dimensional (3D) simulations of dendrite growth using our LB code and generates the geometries of the dendrites. Then, the results were imported into COMSOL (commercial Finite Element Analysis software) to study the effect of Marangoni convection and formation of flow streams in the presence of bubble. Our simulation results show that, in the presence of the bubble, convection near the S/L interface is stronger and the maximum flow velocity is observed near the bubble/liquid interface. The same trends can be seen in PFMI videos as well. The tracer dendrite branches slow down as they distance from the interface and accelerate on their return. The results also showed that the velocity magnitude is larger in front of the bubble in the case when only Marangoni convection is responsible for convection (micro-gravity conditions). We also performed simulations for terrestrial conditions in which free convection due to gravity was the main factor controlling the flow velocity, while Marangoni effect was not significant.

The fluid velocities simulated in COMSOL were imported back to our 3D LBM model for dendritic growth to investigate the effect of induced Marangoni convection on the morphology of dendrites. We observed that the induced Marangoni convection changes the temperature field. The temperature profile was not linear ahead of dendrite tip; the melt near the bubble had a higher temperature. The Marangoni convection is responsible for the relatively higher temperature near the bubble. Also, the growth rate decreases in the dendrites closer to the bubble.

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