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PI Name:	Eshraghi, Mohsen Ph.D.		
Project Title:	Pore-Mushy Zone Interaction during Directional Solidification of Alloys: Three Dimensional Simulation and Comparison with Experiments		
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Comments:			
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COI Name (Institution):	Tewari, Surendra Ph.D. (Cleveland State University) Felicelli, Sergio Ph.D. (University of Akron)		
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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 exploited forefront methods in microscale solidification. We used a methodology based on cellular automaton (CA) and phase field (PF) to determine the interface between phases 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 was 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 can impact the design of improved mushy zone models based on the microstructure information obtained from the direct simulation. The developed knowledge advanced the state of understanding of solidification phenomena in the microscale, contributed to improved numerical predictions of porosity formation, and advanced 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 simulation 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 helped to 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 can 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. This research not only provided 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 was a 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.
	We investigated various enhancements available for the multiphase Lattice Boltzmann (LB) models in order to come up with a reliable scheme to simulate motion and interaction of bubbles during dendritic solidification in binary alloys. The Shan-Chen model, which is the most popular multiphase LB model, was investigated. First, the original Shan-Chen model was studied. A phase separation problem and a contact angle problem were modeled and validated. The interaction of existing bubbles and a dendrite during solidification of a binary alloy was simulated. Although this model can predict the shape of the bubble contacting the solid, it generates a large spurious current. In addition, all of the bubbles tend to merge in an unrealistic manner. Due to the order of magnitude of the spurious current, this model cannot be used to simulate Marangoni effect and natural convection. A realistic equation of state (EOS), middle-range repulsive force, and Exact Difference Method (EDM) force scheme were mixed and implemented to overcome the above-mentioned problems. Although the mixed model reduced the spurious current significantly, the artificial current was still in the same order of magnitude as Marangoni convection. Moreover, the model was unable to reproduce the bubble-dendrite interactions in a meaningful way. By implementing a Phase-Field (PF)-Lattice Boltzmann (LB) model, we eliminated such problems and reduced the spurious current to about 1e-6, which is acceptable. Using the PF-LB model, we simulated bubble-dendrite interactions during directional solidification under Marangoni convection. The results showed that the Marangoni effect tends to remove bubbles from between the dendrites, which favors the growth of more secondary arms as well as a faster growth of the primary arms. 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 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

Task Progress:	branching is enhanced in the vicinity of the bubble. The thermocapillary flow field associated with a bubble in PFMI-15 experiment was investigated. The flow path was tracked by following miniature dendrite branches that made circular routes from the interface, through the bulk liquid, and back, and showed that a flow field that 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. An interesting observation from the PFMI videos was that the tracer dendrite branches invariably accelerated as they approached the solid-liquid interface, We performed large-scale three-dimensional (3D) simulations of dendrite growth using our LB code and generated 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. A 3D Cellular Automaton-Lattice Boltzmann (CA-LB) model was developed to directly investigate the effect of thermocapillary convection induced by bubbles on microstructural evolution during solidification through direct simulations. The large-scale simulations performed with the developed model provided quantitative results about the effects of Marangoni convection on fluid flow, temperature and concentration profiles, growth speed, and orientation of the dendritic microstructure. PFMI experiment and simulation results confirmed that when a large bubble and the solid front are close enough, the induced Marangoni convection can spoil the expected quiescent environment under the microgravity conditions, altering the microstructure. Effect of bubble size was investigated through large-scale simulations of dendrite growth. While no apparent effect on the microstructure was observed for small bubbles, the large bubbles altered the growth rate and tilted the dendrites in the direction of the fluid flow. The simulations provided quantitative information about the effects of Marangoni convection on the microstructure. The results shed light to unexplained observations in the PFMI experiments such as deviation of dendritic array from its original growth direction in the absence of terrestrial convection.
Bibliography Type:	Description: (Last Updated: 12/24/2019)
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