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Project Title:	Pore-Mushy Zone Interaction during Directional Solidification of Alloys: Three Dimensional Simulation and Comparison with Experiments		
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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 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:	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. In order to provide a stable and computationally efficient approach, we are developing multiple-time-step and multiple-grid LB techniques to model the transport phenomena during solidification. To validate our basic dendrite growth model, we measured the dendrite tip growth speed from the PFMI15 test results. The results will be used to verify if our simulation results are in reasonable agreement with the observed behavior.
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