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| **Fiscal Year:** | FY 2021 | **Task Last Updated:** | FY 02/23/2021 |
| **PI Name:** | Asle Zaeem, Mohsen Ph.D. | | |
| **Project Title:** | New Insights on Solid-Liquid Interface Anisotropy Effects on Solidification Patterns of Pure and Alloy Systems in Microgravity | | |
| **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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| **City:** | Golden | **State:** | CO |
| **Zip Code:** | 80401 | **Congressional District:** | 7 |
| **Comments:** | NOTE: PI moved in summer 2018 to Colorado School of Mines from Missouri University of Science and Technology (Ed., 12/10/18) | | |
| **Project Type:** | GROUND,Physical Sciences Informatics (PSI) | **Solicitation / Funding Source:** | 2015-16 Physical Sciences NNH15ZTT001N-15PSI-C: Use of the NASA Physical Sciences Informatics System – Appendix C |
| **Start Date:** | 04/25/2019 | **End Date:** | 09/24/2021 |
| **No. of Post Docs:** | 1 | **No. of PhD Degrees:** | |
| **No. of PhD Candidates:** | 1 | **No. of Master' Degrees:** | |
| **No. of Master's Candidates:** | | **No. of Bachelor's Degrees:** | |
| **No. of Bachelor's Candidates:** | | **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 9/24/2021 per NSSC information (Ed., 4/22/21)<br>NOTE: End date changed to 4/21/2021 per NSSC information (Ed., 9/9/20)<br>NOTE: Period of performance per C-H Su/MSFC is 4/25/2019-4/20/2020 (Ed., 8/14/2019) | | |
| **Key Personnel Changes/Previous PI:** | A postdoc is partially supported to determine the solid-liquid interface energies and their anisotropy for Ti and Al-Cu alloys by molecular dynamics simulations | | |
| **COI Name (Institution):** | | | |
| **Grant/Contract No.:** | 80NSSC19K0569 | | |
| **Performance Goal No.:** | | | |
| **Performance Goal Text:** | | | |

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| **Task Description:** | NOTE: Continuation of "New Insights on Solid-Liquid Interface Anisotropy Effects on Solidification Patterns of Pure and Alloy Systems in Microgravity," grant 80NSSC18K045, when Principal Investigator was affiliated with Missouri University of Science and Technology.<br>The objective of this work is to study and predict the microscale patterns that develop in solidification of pure and alloy systems in microgravity, and investigate and compare the effect of solid-liquid interface anisotropy in microgravity and terrestrial conditions. A multiscale computational framework integrating molecular dynamics simulations and phase-field modeling will be utilized to quantitatively predict solid-liquid interface properties at the nanoscale and use these data to predict solidification patterns at the microscale.<br><br>Solidification of pure Al and Ti, and binary Al-Cu alloys are simulated to study and compare dendritic solidification patterns in microgravity and terrestrial conditions. The data generated by MICAST/CSS (Microstructure Formation in Casting of Technical Alloys under Diffusive and Magnetically Controlled Convective. Conditions/Comparison of Structure and Segregation in Alloys Directionally Solidified in Terrestrial and Microgravity Environments) 6 & 7 will be utilized to validate the computational modeling results.<br><br>The recently developed phase-field finite-element models in Principal Investigator's (PI) research group for predicting dendritic solidification patterns in pure and alloy systems will be modified and implemented in the Idaho National Lab's MOOSE framework (Multiphysics Object-Oriented Simulation Environment) to study and predict three-dimensional microstructures of solidification. The required nanoscale input parameters for phase-field models, such as interface energies and anisotropy of Al-Cu alloys are calculated by MD simulations. It is essential to notice that most of the current mesoscale computational models do not include the actual interface energies and anisotropy coefficients, and only utilize arbitrary values to generate the desired patterns. The main focus of this work will be on studying the effects of solid-liquid interface properties on solidification patterns in microgravity condition; moreover some simulations at terrestrial gravity will be completed to compare the patterns at microgravity and terrestrial conditions. The validation in microgravity condition is particularly essential in order to confidently use the proposed multiscale model to study other pure and alloy materials in microgravity condition and compare their microstructures and segregation regions to those in terrestrial gravity.<br><br>The multiscale computational models that will be developed in this work can be used later to study solidification microstructures of other pure and binary alloys, and can be extended to study ternary alloys and ferrous metals in microgravity; this will result in developing the capability of accurately predicting solidification patterns and microstructures that develop in casting, welding, and laser and/or electron beam additive manufacturing in microgravity. |
| **Rationale for HRP Directed Research:** | |
| **Research Impact/Earth Benefits:** | Since solid-liquid interfacial forces become dominant in the absence of the Earth's gravity, we hypothesize that the proposed solidification phase field-simulations in microgravity conditions will enable us to fundamentally understand and distinguish transport phenomena, defect formation, and microstructural evolution mechanisms in traditional and advanced (e.g., additive) manufacturing processes in Earth's gravity. |
| **Task Progress:** | Solid-liquid (SL) interfacial energy and its anisotropy play a crucial role in solidification pattern formation during alloy solidification. Due the length and time scale limitations of experiments, we used atomistic simulations to determine the values of SL interfacial energy and related anisotropy. The capillary fluctuation method was used for these calculations, and the microstructure evolution and pattern formation during solidification of pure Ti and different Al-Cu binary alloys were studied via multi-phase field modeling.<br>Majority of the phase-field models in the literature for study of solidification considered material properties and phase-field parameters to be independent of the working temperature. We have developed a model where all material properties and model parameters depend on the temperature. As a benchmark example, we have developed an atomistic-informed phase-field model for pure Ti where all the material properties were calculated by atomistic simulations. Temperature-dependent interface energy was determined using the CFM. But this requires obtaining the pressure-temperature phase diagram. We used molecular dynamics simulations using 2NN-MEAM interatomic potentials to calculate the coexistence line for the temperature ranging between -9 to 4 GPa. Then the coexistence line is used to determine the temperature-dependent solid-liquid interface free energy. The mobility as a function of temperature was determined based on the relations for the thin-interface analysis. The mean interface energy decreases by the increase of temperature and MD results were compatible with the analytical relation Thompson-Spaepen (Acta Metallurgica, 1979). The anisotropy parameters change in a way that that as the undercooling increases the {100} orientation becomes the preferred growth direction.<br><br>In comparison to the other phase-field models, the current results are more accurate and closer to the experimental results and analytical models. In order to validate our model, we compared the steady-state solidification rate obtained from the current PF model , the PF model by Karma and Rappel (Physical Review E, 1998) with two sets of experimental data. The results of both PF models are very close to experimental data for undercooling smaller than 200 K. In comparison to the PF model by Karma and Rappel, the current PF model presents a closer prediction to the experimental data as undercooling exceeds 200 K.<br><br>We also studied the solidification microstructures of Al-Cu alloys in different mediums with different heat transfer coefficients (h=0.5, 1.5, 5, and 10 w/cm2K). The atomistic simulations showed that the SL interface free energy decreases by a decrease of temperature or by an increase of solute atom concentration. It was shown that the alloy with 3 at% Cu is very sensitive to change of heat transfer coefficient especially in terms of dendrites pattern. When the heat transfer coefficient is low (h=0.5 w/cm2K) the dendrites are slightly tilted against heat transfer direction. Also, in low heat transfer coefficient a seaweed structure forms in this alloy. By increasing heat transfer, dendrites of Al-3%Cu alloy are aligned with heat transfer direction. On the other hand, dendrites of Al-6%Cu, Al-8.4%Cu, and Al-10.6%Cu are always in the direction of heat transfer direction regardless of heat transfer coefficient. In addition to change of dendrites growth direction in alloy with 3% Cu, dendritic patterns and morphologies noticeably differ with change of heat transfer coefficient in this alloy. When h=0.5 w/cm2K, the primary dendrites split in different places and a seaweed structure was formed. By increasing of h to 10 w/cm2K only columnar morphology was developed in Al-3%Cu alloy. On the other hand, in alloys with higher Cu content not seaweed structure at low heat transfer coefficient (h=0.5 w/cm2K) nor columnar structure at high heat transfer coefficient (h=10 w/cm2K) form. This behavior is related to interactive effects of interfacial energy anisotropy and solute transport phenomena. In higher Cu content concentration gradient ahead of |

growing interface override the effects of interface anisotropy.

Simulation and analytical results of primary dendrite arm spacing (PDAS) and secondary dendrite arm spacing (SDAS) at different heat transfer coefficient were compared and it was indicated that by increasing heat transfer coefficient, PDAS decreases in the all investigated alloys. In this study, the analytical equations which were driven by Dantzig and Rappaz (2016, EPFL press) were used to verify simulation results. It was shown that for a constant cooling condition (constant h value), PDAS is dependent on anisotropy of interfacial energy and concentration of solute atoms. The simulation results and analytical calculation indicated that by increasing SL interfacial energy, PDAS decreases. Also, the results showed that by increasing heat transfer coefficient from 0.5 to 10 w/cm2K, SDAS decreases but this reduction varies by change of Cu content. Also, by increasing Cu content SDAS decreased which indicates that finer microstructures are obtained in higher Cu content. The predicted primary dendrite arm spacing and secondary dendrite arm spacing showed very good agreement with analytical solutions and experimental data.

In this research, we have created an integrated computational scheme capable of quantitative predictions of solid-liquid interfacial effects on solidification patters and microstructures of pure and binary alloys. This quantitative computational framework is also transferrable to study solidification of other metals and alloys.

References

Thompson CV, Spaepen. On the approximation of the free energy change on crystallization. Acta Metallurgica Volume 27, Issue 12, December 1979, p. 1855-1859.

Karma A, Rappel W-J, Quantitative phase-field modeling of dendritic growth in two and three dimensions. Physical Review E, 1998. 57(4): p. 4323-4349.

Dantzig JA, Rappaz M, Solidification: -Revised & Expanded. 2016: EPFL press.

**Bibliography Type:** Description: (Last Updated: 03/23/2022)