Integration of Processing and Microstructure Models for Non-Equilibrium Solidification in Additive Manufacturing

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Introduction

A novel computational framework connecting processing variables with the effects of non-equilibrium solidification in additively manufactured materials is presented in this work. Integration of a physics-based surrogate laser powder bed fusion process model within a high-throughput Calculation of Phase Diagrams (CALPHAD)-based Integrated Computational Materials Engineering (ICME) framework enables non-equilibrium solidification to be modeled as a function of both composition and processing parameters. Solidification cracking susceptibility of additively manufactured materials is predicted as a function of composition, cooling rate, and energy density for the first time. The modeling framework presented in this work can be used to guide alloy design and process optimization for additive manufacturing.

Solidification Cracking in Al-Cu Alloys

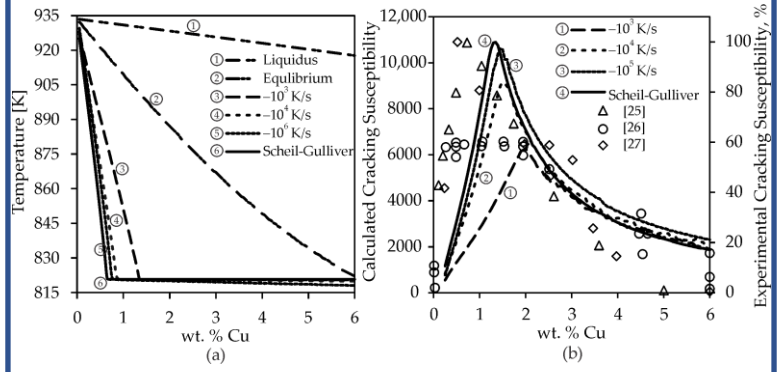

Figure 1. (a) Modeling the effect of cooling rate on the solidus temperature of Al-Cu alloys using the equilibrium, Scheil-Gulliver, and diffusion-controlled transformations (DICTRA) solidification models available in Thermo-Calc software. (b) Solidification cracking susceptibility of Al-Cu alloys calculated by the DICTRA and Scheil-Gulliver models using the Kou solidification cracking susceptibility model. The trend in solidification cracking susceptibility predicted by the model is compared with experimentally observed solidification crack susceptibility data plotted on the secondary y-axis.

Acknowledgement

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Coupling DICTRA with Process Modeling

One-dimensional DICTRA solidification models are implemented using the TC-Python API to enable batch calculations as a function of both processing conditions and composition. A semi-analytic laser powder bed fusion process model is coupled with DICTRA simulations and the Kou solidification cracking susceptibility model to create a CALPHAD-based ICME framework for modeling non-equilibrium solidification in additively manufactured materials. Temperature histories under different processing conditions are used as an input for DICTRA solidification calculations to investigate the relationship between the additive manufacturing process and non-equilibrium solidification.

This approach couples alloy thermodynamics and diffusion with process variables such as laser power, scan speed, and global energy density to model the effect of process parameters on non-equilibrium solidification. The flow chart below shows how the models used in this work are coupled together using the TC-Python application programing interface to create an automated CALPHAD-based ICME framework for modeling solidification in additively manufactured materials.

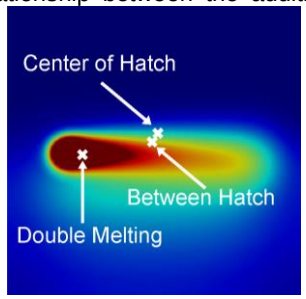

Figure 2. Laser powder bed fusion process model [2].

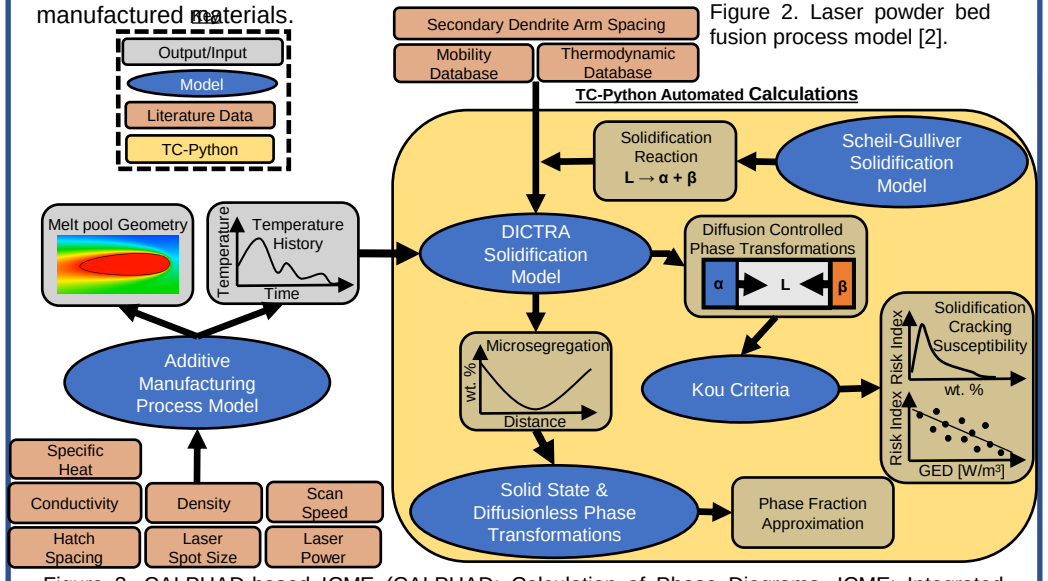

Figure 3. CALPHAD-based ICME (CALPHAD: Calculation of Phase Diagrams, ICME: Integrated Computational Materials Engineering) framework for modeling non-equilibrium solidification of additively manufactured materials. This modeling framework integrates processing and microstructure models for non-equilibrium solidification.

Relating Solidification Cracking to Process Variables

DICTRA is coupled with the laser powder bed fusion process model to predict the solidification cracking susceptibility in stainless steel 316L as a function of energy density. Lower energy density yielded faster cooling rates and higher solidification cracking susceptibility. A location specific relationship was not found.

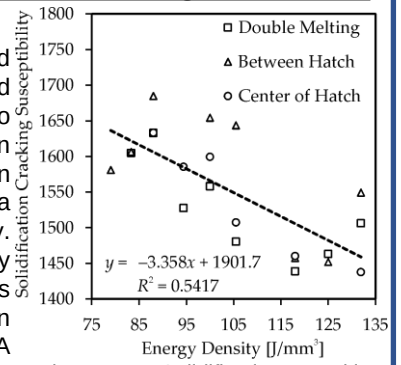

Figure 4. Solidification cracking susceptibility of stainless steel 316L as a function of energy density

Conclusions

- The TC-Python API is used to couple a process model for the LPBF process with a DICTRA solidification model to simulate the process-microstructure relationship between processing variables and non-equilibrium solidification in additively manufactured materials.
- Experimentally observed trends in the solidification cracking susceptibility for the binary Al-Cu system are in good agreement with DICTRA solidification calculations using the model proposed by Kou et al.
- The CALPHAD-based ICME framework predicts a linear relationship between solidification cacking susceptibility and global energy density in additively manufactured stainless steel 316L is predicted using a CALPHAD-based ICME framework.

References

[1] Sargent, N.; Jones, M.; Otis, R.; Shapiro, A.A.; Delplanque, J.-P.; Xiong, W. Integration of Processing and Microstructure Models for Non-Equilibrium Solidification in Additive Manufacturing. *Metals* **2021**, *11*, 570. https://doi.org/10.3390/met11040570

[2] Wolfer, A.J.; Aires, J.; Wheeler, K.; Delplanque, J.-P.; Rubenchik, A.; Anderson, A.; Khairallah, S. Fast solution strategy for transient heat conduction for arbitrary scan paths in additive manufacturing. Addit. Manuf. 2019, 30