ABSTRACT

Laser processing and microstructural evolution in alloy systems involve coupled heat transfer, phase transformation, diffusion, interfacial reactions, and meltpool dynamics. In this dissertation, the laser-microstructure ($\mathscr{L}$-$\mathscr{M}$) interface is treated as a dynamic region where thermal history, composition, free-energy landscape, and morphology evolve together. The main objective is to represent, quantify, compress, reconstruct, and predict this interface using thermodynamically informed computational and data-driven models.

The dissertation develops a computational framework based on phase-field modeling, thermodynamic tensor representation, and physics-informed machine learning. Across the studied alloy systems, microstructural evolution is analyzed through phase-field simulations and represented using physically meaningful descriptors. Building on these simulations, this evolution is further encoded as high-dimensional tensor data, enabling tensor sparsification, decomposition, and reconstruction while preserving essential morphological and interfacial information. This establishes the **Thermodynamic Tensor Representation** as a compact and physically meaningful form for storing and reconstructing simulation-based microstructure data.

The second part extends the framework toward **laser-processed alloy systems**. In the multicomponent $Cu_x(Ti\text{-}6Al\text{-}4V)_y$ system, finite-element heat-transfer simulations and phase-field modeling are used to describe laser-induced Ti_2Cu intermetallic growth in the matrix. In the *Ti-Au* system, a non-isothermal multiphase-field model is developed to resolve meltpool formation, Ti_3Au intermetallic evolution, interdiffusion, and the interaction between thermal and chemical fronts. The model includes temperature- and composition-dependent free-energy functions, KKS-type phase-equilibrium constraints, and coupled heat-transfer and fluid-flow effects. In the unary Au system, different laser beam profiles and free-energy descriptions are compared to study their influence on meltpool morphology, phase evolution, and Marangoni-driven flow.

The final part develops **machine learning models for computational acceleration**. Conv-LSTM models predict multi-generational microstructural evolution in binary alloy systems, including Pd-Rh and Cu-Mn examples, while U-Net-based MicroTwin and FlowTwin models predict phase and velocity fields from temperature data in laser-processed Au. The predictions are evaluated using interface-sensitive descriptors such as microstructural similarity, shape index, blob detection, meltpool geometry, and velocity fields.

Overall, the dissertation shows that the $\mathscr{L}$-$\mathscr{M}$ interface can be described through a thermodynamically grounded tensor framework supported by multiphysics simulations and physics-informed learning models. The developed methodology provides a route **Toward Digital Twin** construction for laser-processed multicomponent alloys.