Silesian University of Technology

Faculty of Mechanical Engineering

Department of Engineering Materials and Biomaterials

EXTENDED ABSTRACT

Towards Digital Twins for Quantifying Laser-Microstructure Interface in Multicomponent Alloys Using Thermodynamic Tensor Model

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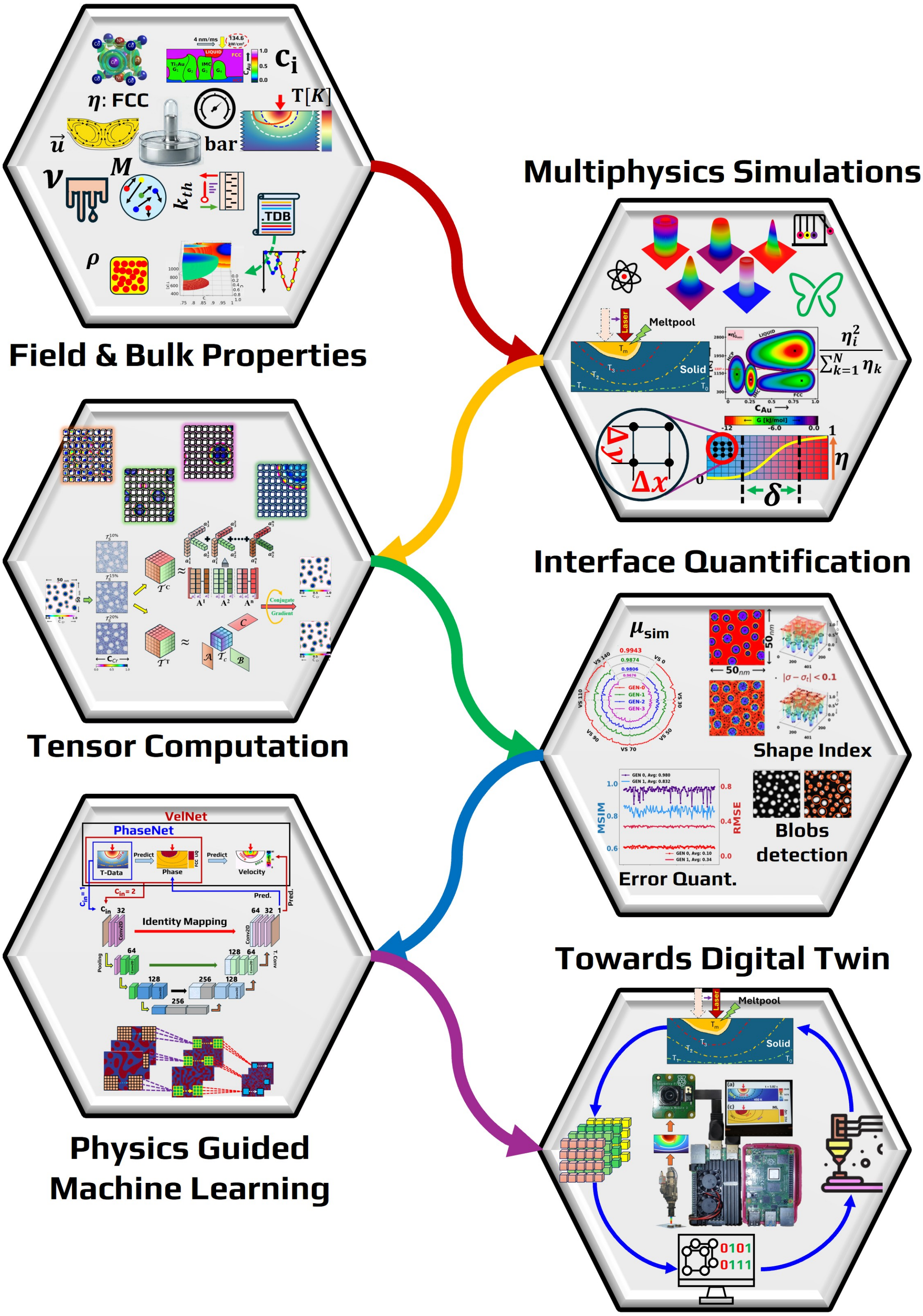
GRAPHICAL ABSTRACT



EXTENDED ABSTRACT

1 Scope of the dissertation

Laser-based additive manufacturing and laser surface processing of metallic alloys involve highly coupled thermal, chemical, phase-transformation, and fluid-flow phenomena. During laser-material interaction, localized heat input produces strong thermal gradients, rapid melting and solidification, interdiffusion, interfacial reactions, meltpool flow, and phase evolution. In multicomponent alloys, these processes become more complex because the microstructural response is controlled not only by the imposed laser-processing parameters, but also by the alloy composition, the local thermodynamic stability of phases, the diffusion kinetics of elements, and the evolution of interfaces. The scope of this dissertation is the computational representation, quantification, compression, reconstruction, and prediction of the laser-microstructure ($\mathscr{L}$-$\mathscr{M}$) interface in alloy systems. In this work, the $\mathscr{L}$-$\mathscr{M}$ interface is not treated only as a geometrical boundary. Instead, it is considered a dynamic region where thermal history, phase state, composition, free-energy landscape, diffusion, interfacial reactions, and meltpool flow evolve together. The dissertation develops a framework that combines thermodynamically informed phase-field modeling, tensor-based representation of microstructural evolution, and physics-informed machine learning. These components are integrated as a route toward Digital Twin development for laser-processed multicomponent alloys.

The scientific scope is developed through five thematically related published articles. Article I [1] establishes the tensor-based representation and reconstruction of phase-field-generated microstructural evolution data in a Ti-Cr alloy system. Article II [2] combines experiments, finite-element thermal analysis, and phase-field modeling to describe laser-induced Ti_2Cu intermetallic growth in a $Cu_x(\text{Ti-6Al-4V})_y$ system. Article III [3] develops a Conv-LSTM framework for multi-generational prediction of microstructural evolution directly in manifest space. Article IV [4] develops a non-isothermal multiphase-field model for meltpool and Ti_3Au intermetallic grain interaction in a Ti-Au system. Article V [5] develops a phase-field-informed U-Net framework for learning meltpool morphology and velocity fields under different laser beam profiles and thermodynamic free-energy descriptions in unary Au.

Together, these studies define a computational route for describing the $\mathscr{L}$-$\mathscr{M}$ interface from three complementary perspectives. **First, multiphysics phase-field modeling** provides a physically grounded description of thermal, chemical, phase, and flow fields. **Second, tensor representation** enables high-dimensional microstructural data to be stored, compressed, reconstructed, and treated as a structured object. **Third, machine learning models** enable rapid prediction of microstructural and meltpool evolution while preserving spatial and interfacial information. The dissertation therefore addresses both the physical problem of laser-induced microstructural evolution and the computational problem of representing and predicting such evolution in a scalable manner.

2 Dissertation objectives

The main objective of the dissertation is **to develop a thermodynamically informed computational framework for quantifying and predicting the laser-microstructure interface in multicomponent alloy systems by integrating phase-field modeling, thermodynamic tensor representation, and physics-informed machine learning**.

This objective is motivated by the need to describe microstructural evolution during laser processing not only through isolated scalar outputs, such as maximum temperature or meltpool depth, but through full spatio-temporal fields. The dissertation therefore focuses on field variables such as temperature, phase distribution, composition, order parameters, meltpool velocity, intermetallic growth, and interface morphology. These variables are resolved through multiphysics simulations, encoded in tensor form, and used as physically meaningful data for prediction.

2.1 Specific objectives and thesis of the dissertation

Based on this main objective, the dissertation specifically aims to model laser-induced phase separation, interdiffusion, intermetallic growth, meltpool evolution, and phase transformation using phase-field and finite-element methods; to represent the resulting spatio-temporal microstructural fields as tensor data for compression, reconstruction, and analysis; to quantify interfacial and morphological features using similarity, shape, meltpool, intermetallic-thickness, Lewis-number, and positional-time-lag descriptors; and to develop machine learning models capable of predicting microstructure, phase state, and meltpool velocity directly in the spatial domain. The **thesis of the dissertation is that thermodynamically consistent multiphysics simulation data, when encoded through tensor representation and used for manifest-space machine learning, can preserve and predict the spatial, temporal, and interfacial characteristics of laser-induced microstructural evolution.** This integrated approach provides a scalable basis for Digital Twin-oriented modeling of laser-microstructure interaction in multicomponent alloy systems.

3 Description of the research subject

3.1 Laser-Microstructure ($\mathscr{L}$-$\mathscr{M}$) interface

The research subject of the dissertation is the $\mathscr{L}$-$\mathscr{M}$ interface in alloy systems. This interface is created and transformed during laser processing, where a moving heat source generates a localized thermal field and drives the formation, growth, dissolution, or motion of phases. In the context of this dissertation, the interface is understood as a coupled physical and informational object. Physically, it is the region where phase boundaries, composition gradients, thermal gradients, and interfacial reactions are concentrated. Informationally, it is the region whose morphology and dynamics must be preserved in computational datasets and learned by predictive models. In laser processing, the thermal field is the first field directly controlled by external process parameters such as laser power, irradiance, scan speed, beam radius, and beam shape. However, the microstructure does not respond instantaneously to the thermal field. Phase evolution, chemical diffusion, intermetallic formation, and meltpool motion may lag behind the thermal front. Therefore, a key part of the dissertation is the quantification of differences between the thermal front and the phase or chemical diffusion front. This lead-lag behavior between thermal and phase fronts, quantified using Lewis number and positional time lag, is shown in Figure 1.

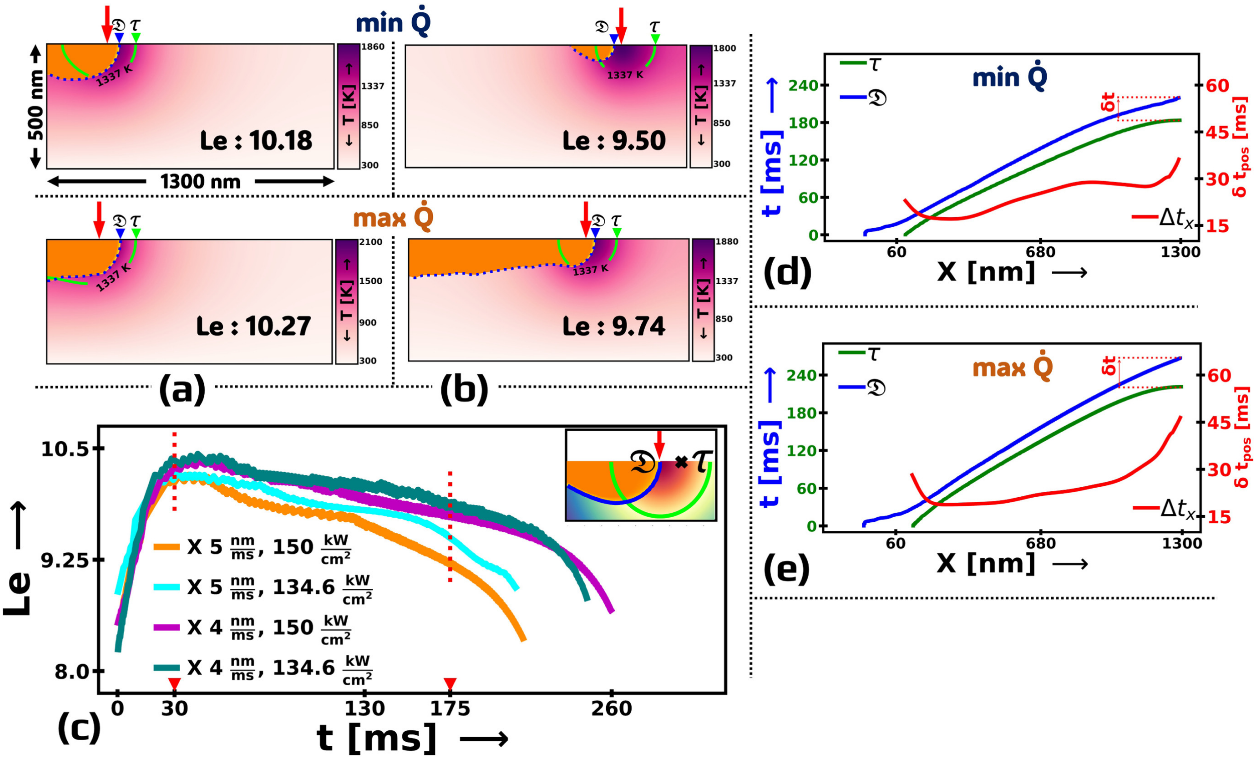


Figure 1. Lead-lag dynamics between thermal and phase fronts, quantified using Lewis number and positional time lag [4].

3.2 Multiphysics phase-field modeling

The phase-field method provides the main physics-based modeling foundation of the dissertation. It allows the evolution of phases and interfaces to be described using continuous field variables. Conserved variables, such as composition, are governed by convection-diffusion equations, while non-conserved variables, such as order parameters, are governed by Allen-Cahn-type equations. The driving force for evolution is the free energy of the system, which depends on composition, temperature, phase state, and interfacial energy.

In the Ti-Cr alloy system, phase-field simulation is used to generate microstructural evolution data associated with phase separation and elasto-chemical effects. The resulting microstructural data are treated as high-dimensional tensors for sparsification, decomposition, and reconstruction. In the $Cu_x(Ti\text{-}6Al\text{-}4V)_y$ system, finite-element heat-transfer analysis is coupled with phase-field modeling to investigate the thermodynamic conditions favorable for Ti_2Cu intermetallic growth. In the Ti-Au system, a non-isothermal multiphase-field model is developed to study the interaction among meltpool formation, interdiffusion, Ti_3Au intermetallic grain growth, heat transfer, and fluid flow. In the unary Au system, a phase-field model is coupled with heat transfer and meltpool flow to compare the effects of Gaussian, Flat-Top, Ring, and Bessel laser beam profiles.

A common feature across these studies is the use of temperature-dependent and, where needed, composition-dependent thermodynamic information. The free-energy landscape is not treated as a purely mathematical convenience, but as the physical driving force that determines phase stability and interface motion. The overall methodological relationship among thermodynamics, multi-physics phase-field modeling, tensor representation, machine learning, and Digital Twin development is summarized in Figure 2.

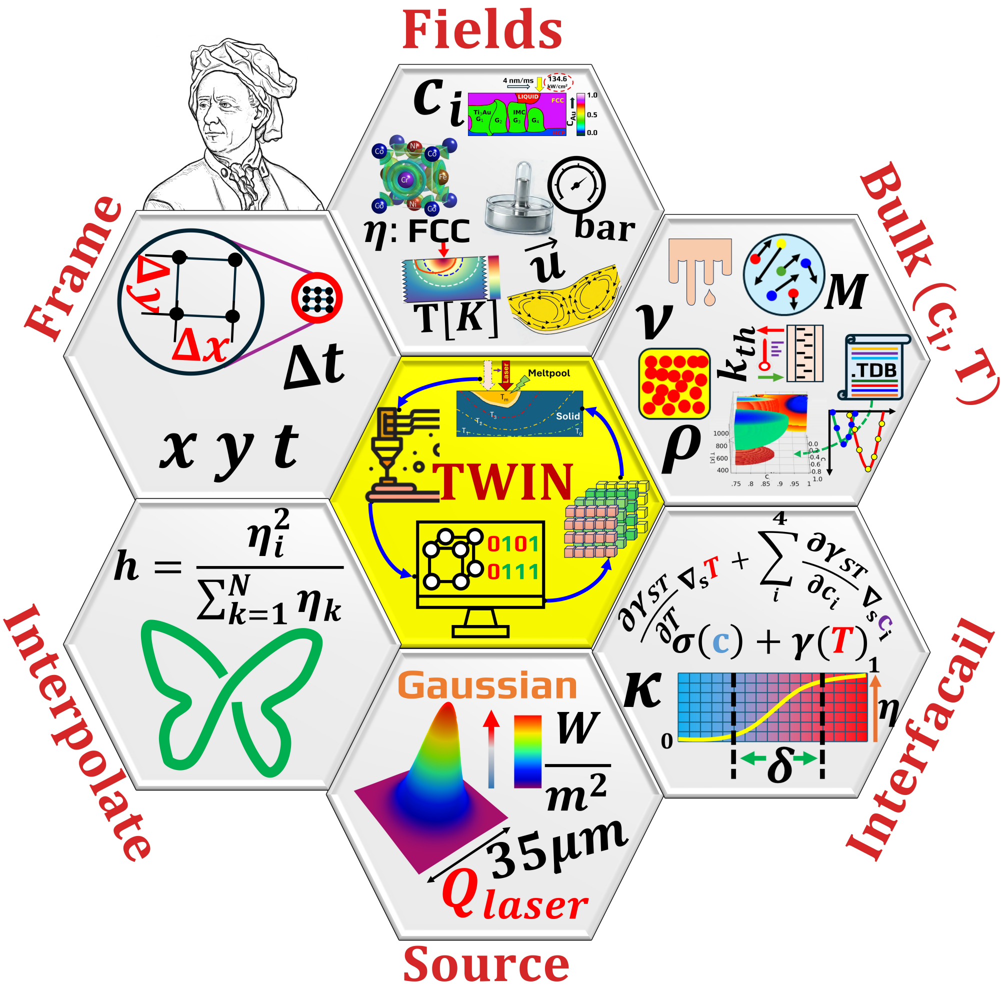


Figure 2. Multiphysics phase-field workflow linking thermodynamics, tensor modeling, machine learning, and virtual Digital Twin development.

3.3 Thermodynamic tensor representation

The Thermodynamic Tensor Model is the representational component of the dissertation. Phase-field simulations generate large spatio-temporal datasets that are difficult to store, transfer, reconstruct, and reuse. These datasets contain spatio-temporal field variables, including phase state, composition, temperature, strain, or velocity. Treating them as ordinary image sequences or isolated arrays does not fully exploit their multidimensional structure.

Tensor representation addresses this limitation by encoding microstructural evolution into structured multidimensional arrays. In Article I, phase-field-generated Ti-Cr microstructural evolution data were transformed into dense tensors and then sparsified. Tensor decomposition and reconstruction methods, including Canonical Polyadic and Tucker decomposition, were evaluated to determine whether microstructural morphology and interfacial information could be recovered from sparse data. This tensor sparsification, decomposition, and reconstruction workflow is shown in Figure 3.

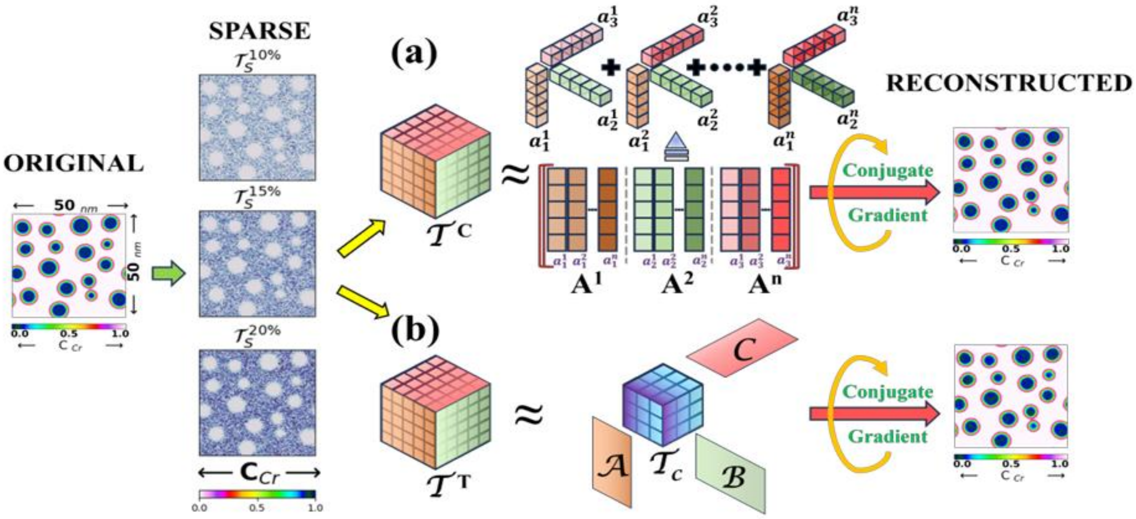


Figure 3. Tensor sparsification, decomposition, and reconstruction of phase-field microstructural evolution data **[1]**.

The results showed that tensor-based reconstruction can significantly reduce data size while preserving essential microstructural information. In the context of the dissertation title, the term **Thermodynamic Tensor Model** refers to the broader idea that thermodynamic and microstructural fields can be represented as tensorial objects retaining spatial, temporal, and physical relationships. This makes large simulation outputs portable and learnable for Digital Twin development. Thus, the tensor model acts as a bridge between high-fidelity physics-based simulations and scalable data-driven prediction.

3.4 Physics-informed machine learning

The final research component is physics-informed machine learning for microstructure and meltpool prediction. Conventional machine learning approaches often remove interface-level information and make the predictions difficult to interpret physically. This dissertation instead emphasizes **manifest-space learning**, in which the model predicts spatial microstructural fields directly. Article III develops a Conv-LSTM framework for multi-generational prediction of microstructural evolution. The model uses phase-field-generated image sequences and predicts future frames while preserving interfacial morphology. The multi-generational prediction strategy, where simulated frames are progressively replaced by predicted frames, is shown in Figure 4. The predictions are evaluated using similarity metrics, shape index analysis, blob detection, and histogram-based descriptors to verify interface-level preservation.

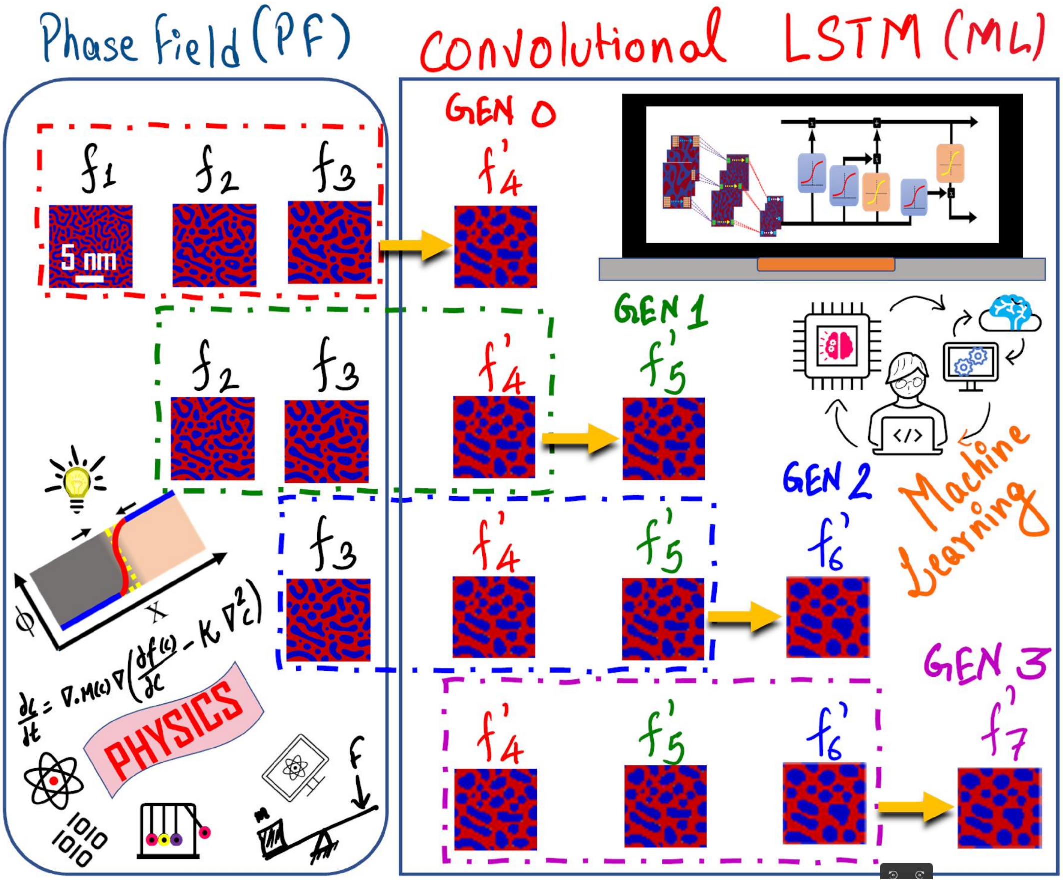


Figure 4. Multi-generational microstructure prediction using the Conv-LSTM framework [3].

Article V develops a two-stage U-Net-based framework for laser meltpool prediction. The first model, **MicroTwin**, predicts phase distribution from temperature input. The second model, **FlowTwin**, predicts velocity fields using temperature and predicted phase information. This creates a physics-informed prediction chain in which the temperature field is connected to phase state and meltpool flow. The virtual Digital Twin workflow based on MicroTwin and FlowTwin is shown later in Figure 5.

4 Main methodology

The methodology of the dissertation combines **four levels of modeling and analysis**.

The first level is multiphysics simulation. Phase-field models are used to resolve phase separation, phase transformation, interfacial motion, and intermetallic growth. Heat-transfer equations describe the transient temperature field under laser irradiation, while fluid-flow equations describe meltpool motion where the liquid phase is present. Thermodynamic data are incorporated through free-energy functions, phase diagrams, temperature-dependent material properties, and fitted or database-derived expressions.

The second level is data representation. Simulation outputs are converted into structured spatio-temporal data. In the Ti-Cr study, microstructural evolution data are stored in tensor form and sparsified. CP and Tucker decomposition are then used to reconstruct dense microstructural information from reduced datasets.

The third level is interface-sensitive quantification. Instead of evaluating simulation and prediction results only by global measures, the dissertation uses descriptors that focus on morphology and interface dynamics. These include microstructural similarity index, root mean squared error, blob detection, shape index, phase area, meltpool width and depth, intermetallic layer thickness, maximum temperature, meltpool velocity, Lewis number, and positional time lag.

The fourth level is machine learning prediction. Conv-LSTM models are trained to forecast microstructural evolution across multiple generations, while U-Net models are trained to predict phase and velocity fields from temperature data. These learned models are used as accelerated surrogates trained on thermodynamically and physically informed simulation data.

5 Main results and discussion

5.1 Tensor reconstruction of microstructural evolution

Article I demonstrated that phase-field-generated microstructural evolution data can be represented in tensor form, compressed, and reconstructed while retaining essential morphological information. In the Ti-Cr alloy system, phase separation was simulated using the phase-field method, and the resulting spatio-temporal data were converted into high-dimensional tensors. Sparsification was then applied, followed by reconstruction using CP and Tucker decomposition methods.

The results showed that the original phase-field dataset could be substantially reduced while preserving microstructural morphology. Tucker decomposition performed better than CP decomposition in retaining microstructural similarity and elastic deformation-related features. The study achieved a 28-fold reduction in data size while preserving the essential structure of the microstructure. This supports the use of tensor representation as a compact and reconstructable data form for microstructure informatics and Digital Twin-oriented workflows.

5.2 Laser-induced Ti_2Cu intermetallic growth in Cu_x(Ti-6Al-4V)$_y$

Article II addressed laser surface alloying of Ti-6Al-4V with Cu and the formation of Ti_2Cu intermetallic compounds. The study combined experimental observations with computational heat-transfer and phase-field modeling. The finite-element model described the transient thermal history generated during laser processing, while the phase-field model described intermetallic growth in the Ti-6Al-4V matrix.

The computational results showed that Ti_2Cu growth is thermodynamically favorable under the simulated thermal conditions. The local temperature field provides the thermal exposure required for interdiffusion and intermetallic formation, while the phase-field results showed heterogeneous grain growth influenced by curvature effects between adjacent grains. In the context of the dissertation, this study provides an experimentally connected example of $\mathscr{L}$-$\mathscr{M}$ interaction in a multi-component material system.

5.3 Manifest-space prediction of microstructural evolution

Article III developed a Conv-LSTM framework for predicting microstructural evolution directly in the spatial domain. The model was trained using phase-field-generated microstructural sequences. Unlike latent-space approaches, the Conv-LSTM framework operated on image-like microstructural fields, preserving the spatial arrangement of interfaces.

The model enabled multi-generational prediction, where predicted frames were progressively used as inputs for forecasting later generations. The predicted microstructures showed high similarity with phase-field ground truth results, with microstructural similarity indices of 0.994, 0.987, 0.980, and 0.967 for four consecutive generations. Shape index analysis, blob detection, histogram comparison, and similarity metrics confirmed that the predicted microstructures retained interface-level features. The framework was also applied to Pd-Rh and Cu-Mn alloy systems, demonstrating its use for time-aware microstructure prediction in engineering alloy examples.

5.4 Non-isothermal multiphase-field modeling

Article IV developed a non-isothermal multiphase-field model for the Ti-Au system, incorporating heat transfer, phase-field evolution, interdiffusion, meltpool formation, Ti_3Au intermetallic growth, and fluid-flow effects. Temperature- and composition-dependent free-energy functions were used to describe the thermodynamic stability of HCP, FCC, LIQUID, and Ti_3Au phases.

The results showed that laser irradiance and scan speed strongly influence meltpool geometry and intermetallic growth. At higher heat flux conditions, the meltpool depth increased from 158 nm to 180 nm, while the Ti_3Au intermetallic layer thickness reached 364 nm, corresponding to a 25% increase compared with lower irradiance conditions. A key result was the identification of lead-lag behavior between thermal and phase fronts, shown earlier in Figure 1. This demonstrated that temperature contours alone are insufficient to describe microstructural interface motion during laser processing.

5.5 U-Net-based virtual Digital Twin framework

Article V extended the dissertation toward machine-learning-assisted Digital Twin development. The study compared laser processing of unary Au under four beam profiles: Gaussian, Flat-Top, Ring, and Bessel. Two thermodynamic free-energy descriptions were considered: a fitted formulation and a TDB-based thermodynamically consistent formulation. The phase-field simulations resolved temperature distribution, phase evolution, meltpool morphology, and velocity fields.

The comparison showed that beam profile and free-energy formulation strongly influence maximum temperature, meltpool geometry, phase evolution, and meltpool flow. The TDB-based free-energy formulation reproduced the lead-lag behavior between thermal and phase fronts more clearly than the fitted formulation, reinforcing the importance of thermodynamic consistency in non-isothermal phase-field modeling.

The simulation data were used to train U-Net-based surrogate models. MicroTwin predicted phase evolution from temperature input with training, validation, and testing accuracies of 0.9992, 0.9989, and 0.9979, respectively. FlowTwin predicted meltpool velocity using temperature and phase information, achieving a test R^2 value of 0.999. This framework connects thermodynamically informed phase-field simulations with rapid prediction of phase and velocity fields, establishing a route toward Digital Twin-based representation of the laser-microstructure interface, as summarized in Figure 5.

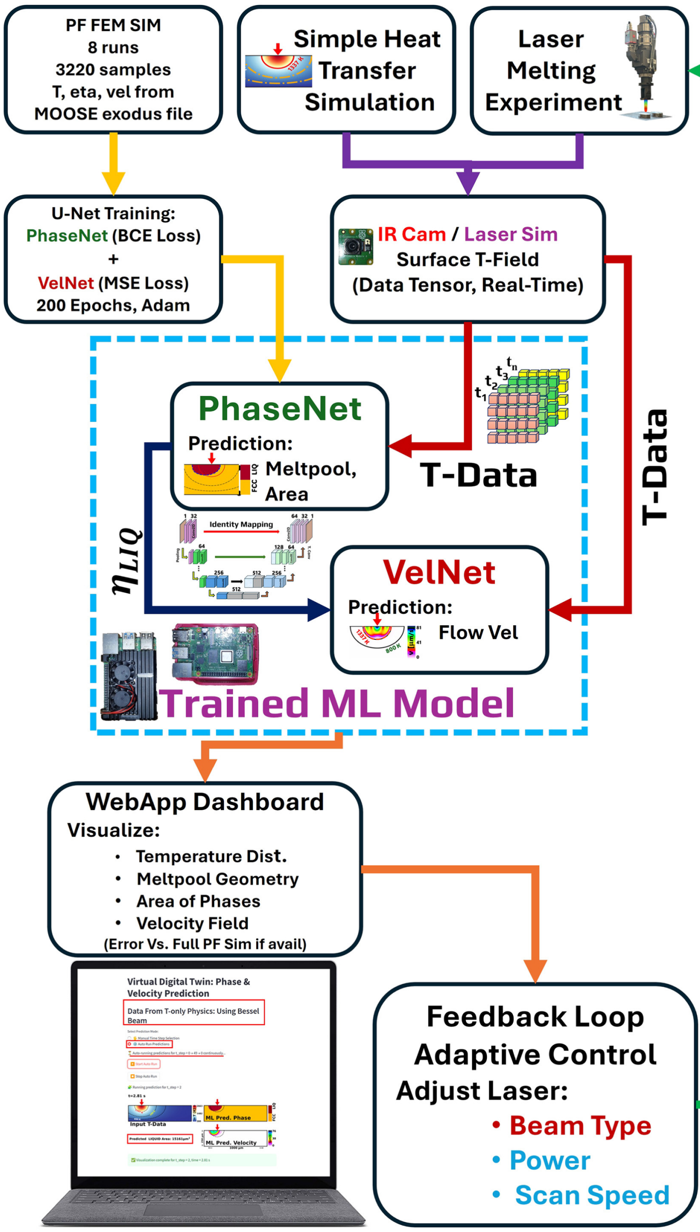


Figure 5. Virtual Digital Twin framework using MicroTwin and FlowTwin for meltpool phase and velocity prediction [5].

6 Author's publications and contribution details

The doctoral dissertation is based on five thematically related scientific publications. In Articles I, III, IV, and V, the author of the dissertation is the **first** and **corresponding author**. In these publications, the author carried out the main scientific and computational work, including conceptualization, model development, simulation design, code implementation, data generation, formal analysis, validation, visualization, interpretation of results, and preparation of the original manuscript draft. The supervision, project administration, funding acquisition, and final scientific review were provided by the co-authors. In Articles II, the author's contribution was focused on the computational part of the study, particularly phase-field simulation, code development, visualization, formal analysis, and interpretation of the numerical result.

Article I

U. Subedi, N. Moelans, T. Tański and A. Kunwar, "Rapid portabilization of elasto-chemical evolution data for dental Ti-Cr alloy microstructure through sparsification and tensor computation." *Scripta Materialia*, 2024, [1]. DOI: https://doi.org/10.1016/j.scriptamat.2024.116027.

Author's contribution – 71%

The author of the dissertation was the **first and corresponding author** of this publication, with a declared contribution of 71%. The author was responsible for the main scientific concept of the work, including the idea of representing phase-field-generated Ti-Cr microstructural evolution data in tensor form and applying sparsification, tensor decomposition, and reconstruction techniques for microstructure informatics. The author developed and performed the phase-field simulations of Ti-Cr phase separation, prepared the microstructural datasets, converted the simulation results into dense and sparse tensor representations, implemented the tensor decomposition and reconstruction workflow, and carried out the comparison between CP and Tucker decomposition methods. The author also performed the formal analysis and validation of reconstructed microstructures using quantitative descriptors such as microstructural similarity, RMSE, blob detection, and shape index analysis. The visualization of the phase-field results, tensor workflow, reconstructed microstructures, and quantitative comparison plots was prepared by the author. The author interpreted the results in relation to elastic deformation preservation, microstructural morphology reconstruction, and the potential use of tensor-compressed microstructure data in digital manufacturing. The original manuscript draft was written by the author.

Article II

H.B. Mamo, **U. Subedi**, T. Poloczek, M. Adamiak, A.N.S. Appiah, M. Skonieczna, P.M. Nuckowski, Y. Geng, B. Haldar, and A. Kunwar "Prototyping Ti2Cu intermetallic grain growth heterogeneously in Ti6Al4V matrix through laser additive manufacturing" *Materials & Design*, 2024, [2]. DOI: https://doi.org/10.1016/j.matdes.2024.113312.

Author's contribution – 16%

The author of the dissertation contributed 16% to this publication. The author's contribution was focused on the computational modeling and numerical analysis part of the work. The author developed and implemented the phase-field simulation framework used to describe Ti_2Cu intermetallic compound growth in the Ti-6Al-4V matrix under laser-processed conditions. This included code development, model implementation, simulation execution, visualization of intermetallic grain evolution, and formal analysis of the computational results. The author contributed to the interpretation of the thermodynamic and phase-field aspects of the study, particularly the relationship between free-energy driving force, interdiffusion, curvature effects, and heterogeneous Ti_2Cu grain growth. The author also contributed to validation and visualization of the numerical results and participated in manuscript review and editing. The experimental laser surface alloying, microstructural characterization, microbiological testing, and experimental analysis were carried out by the other co-authors. Thus, the author's contribution in this article was primarily the computational phase-field modeling and analysis of the intermetallic growth mechanism.

Article III

U. Subedi, N. Moelans, T. Tański and A. Kunwar, "Foretelling microstructural interface with multi-generational convolutional-LSTM framework." *Engineering with Computers*, 2025, [3]. DOI: https://doi.org/10.1007/s00366-025-02117-z.

Author's contribution – 72%

The author of the dissertation was the **first and corresponding author** of this publication, with a declared contribution of 72%. The author was responsible for the main concept of developing a manifest-space machine learning framework for forecasting microstructural evolution using phase-field-generated data. The author designed the computational workflow, generated the phase-field simulation datasets for binary alloy phase decomposition, extracted and processed the spatio-temporal image sequences, and prepared the training, validation, and testing datasets for the neural network models. The author developed and trained the Conv-LSTM architectures used for multi-generational microstructure prediction. This included the design and comparison of different input-output model structures, implementation of the training workflow, prediction of successive microstructural generations, and evaluation of the trained models. The author carried out the full formal analysis of the predicted microstructures using similarity metrics, histogram comparison, blob detection, and shape index analysis to verify whether the machine-learning predictions preserved interface-level information. The author also applied the trained model to engineering alloy examples and interpreted the results in the context of computational reducibility and interface-aware microstructure prediction. All major visualizations, including neural network workflow diagrams, phase-field data preparation schemes, prediction results, and quantitative validation plots, were prepared by the author. The original manuscript draft was written by the author.

Article IV

U. Subedi, N. Moelans, T. Tański and A. Kunwar, "A non-isothermal multi-phase field approach to model the meltpool and IMC grains interaction in Ti-Au material" *Computational Materials Science*, 2025, [4]. DOI: https://doi.org/10.1016/j.commatsci.2025.113875.

Author's contribution – 70%

The author of the dissertation was the **first and corresponding author** of this publication, with a declared contribution of 70%. The author was responsible for developing the main research concept and computational framework for modeling laser-induced meltpool and Ti_3Au intermetallic grain interaction in a Ti-Au material system. The author formulated and implemented the non-isothermal multiphase-field model, including temperature- and composition-dependent free-energy descriptions, phase-field equations, heat-transfer coupling, meltpool representation, and interdiffusion-driven IMC growth. The author performed the computational simulations under different laser irradiance and scan-speed conditions and carried out the formal analysis of phase evolution, meltpool geometry, intermetallic growth, phase stability, and free-energy variation. The author also developed and applied the quantitative analysis of lead-lag behavior between thermal and phase fronts using Lewis number and positional time lag. These analyses were used to interpret the difference between heat-flow propagation and chemical or phase-front evolution during laser processing. The author prepared the simulation datasets, performed validation and numerical interpretation, and created the visualizations of the computational domain, phase evolution, thermal fields, meltpool behavior, IMC growth, and lead-lag metrics. The original manuscript draft was written by the author.

Article V

U. Subedi, A. Bhattarai, N. Moelans, T. Tański and A. Kunwar, "Spatiotemporally learning the morphological and dynamic features of Au meltpool under different heat source types with phase-field informed U-Net framework" *Computational Materials Science*, 2025, [5].

DOI: https://doi.org/10.1016/j.commatsci.2025.114456.

Author's contribution – 60%

The author of the dissertation was the **first and corresponding author** of this publication, with a declared contribution of 60%. The author developed the main scientific concept of combining phase-field simulations with U-Net-based machine learning for predicting laser-induced meltpool morphology and velocity fields. The author formulated and implemented the phase-field simulation framework for unary Au under different laser beam profiles, including Gaussian, Flat-Top, Ring, and Bessel heat sources. The author also implemented and compared two free-energy formulations, namely the fine-tuned expression and the TDB-based thermodynamic expression, to investigate their influence on phase evolution and lead-lag behavior between thermal and phase fronts. The author generated the simulation datasets, analyzed temperature fields, phase evolution, meltpool morphology, meltpool velocity, beam-profile-dependent thermal response, and differences between free-energy formulations. The author contributed to the development of the phase-field-informed machine learning workflow in which the primary network predicts phase/meltpool morphology from temperature input, and the secondary network predicts velocity fields using temperature and phase information. The author carried out the formal analysis, validation, interpretation, and visualization of the simulation and machine-learning results. The author also prepared the Digital Twin-oriented interpretation of the work, connecting the trained U-Net models with the possibility of rapid phase and velocity prediction from thermal input data. The figures, computational workflow, simulation-result visualizations, free-energy comparison plots, beam-profile analyses, and Digital Twin framework diagrams were prepared under the author's lead. The original manuscript draft was written by the author.

Overall, the author's contribution across the five publications can be summarized as the development of a connected computational framework for laser-microstructure interface quantification. The author performed the principal work in phase-field modeling, thermodynamic implementation, tensor-based microstructure representation, simulation-data generation, machine-learning model development, quantitative validation, and scientific visualization. The supervisory, funding, project-administration, and review-related roles were provided by the co-authors. The combined contribution establishes the scientific foundation of the dissertation, linking thermodynamically consistent multiphysics simulations, tensor computation, and physics-informed machine learning for Digital Twin-oriented modeling of laser-processed alloy systems.

7 Main conclusions

The dissertation shows that the laser-microstructure interface in alloy systems can be described as a coupled thermodynamic, kinetic, morphological, and informational object. The interface is governed by the interaction of thermal history, composition, free-energy landscape, diffusion, interfacial reactions, and meltpool flow. Therefore, accurate prediction of laser-induced microstructure evolution requires models that preserve the coupling among these fields.

The first main conclusion is that thermodynamically informed phase-field models can resolve important mechanisms of laser-induced interface evolution. In the $Cu_x(\text{Ti-6Al-4V})_y$ and Ti-Au systems, the formation and growth of intermetallic phases were shown to depend on local thermal exposure, thermodynamic stability, diffusion kinetics, and interface morphology. In the Au system, the comparison of free-energy descriptions showed that the thermodynamic driving-force formulation can strongly influence the predicted relation between thermal and phase fronts.

The second main conclusion is that the thermal front and the microstructural phase front should not be assumed to be identical. The Ti-Au and Au studies showed that phase evolution can lag behind the thermal field. This behavior was quantified using Lewis number and positional time lag. The result is important because it demonstrates that temperature fields alone are insufficient for describing microstructure evolution during laser processing.

The third main conclusion is that tensor representation provides a compact and physically meaningful way to handle large microstructural datasets. The Ti-Cr study showed that phase-field simulation data can be sparsified, decomposed, and reconstructed with significant data reduction while preserving microstructural morphology and interface information. This supports the use of thermodynamic tensor representation as a foundation for portable microstructure informatics.

The fourth main conclusion is that machine learning can predict microstructural evolution directly in manifest space when trained on physically meaningful simulation data. The Conv-LSTM framework predicted multi-generational microstructural evolution with high similarity to phase-field results, while preserving interface-level morphology. The U-Net-based MicroTwin and FlowTwin models connected temperature fields to phase and velocity predictions, enabling rapid surrogate modeling of meltpool behavior.

The fifth main conclusion is that the integration of multiphysics modeling, thermodynamic tensor representation, and physics-informed machine learning provides a practical route toward Digital Twin development for laser-processed multicomponent alloys. The dissertation does not present a complete industrial Digital Twin, but it establishes the necessary computational elements: physics-based simulation, structured data representation, interface-sensitive quantification, and fast predictive modeling.

8 Future outlook

The framework developed in this dissertation can be extended toward larger simulation domains, longer processing times, broader process windows, and more complex alloy systems. A major future direction is the development of composition-aware Digital Twin models for high-entropy alloys, where microstructural response is governed not only by laser parameters but also by composition-dependent thermodynamics and transport properties. Future work should also integrate simulation-driven models with experimental sensing, and active learning. Combining thermodynamic tensor representation with experimental data could improve the robustness of Digital Twin systems, while tensor reconstruction errors and interface descriptors could guide the selection of new phase-field simulations. In this way, the developed framework provides a basis for flexible, composition-aware, and predictive tools for laser processing of multicomponent alloys.

REFERENCES

Constituent publications forming the scientific framework of the dissertation:

[1] U. Subedi, N. Moelans, T. Tański, A. Kunwar, Rapid portabilization of elasto-chemical evolution data for dental Ti-Cr alloy microstructure through sparsification and tensor computation, Scripta Materialia 244 (2024) 116027. doi:10.1016/j.scriptamat.2024.116027.
URL https://www.sciencedirect.com/science/article/pii/S1359646224000629

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