Attention-guided surrogate reconstruction of multicomponent phase-field simulations for laser-processed CoCrFeNi

Upadesh Subedi[1], Nele Moelans[2], Tomasz Tański[1], Anil Kunwar[1]

1 Politechnika Śląska

2 KU LEUVEN

Introduction

Motivation

- Multiphysics laser-processing: **CoCrFeNi** (HEA)
- Phase Field (PF) simulations are accurate but costly
- High-dimensional CALPHAD data
- Need for real-time Digital Twin prediction

Objective

Physics Guided AI pipeline

- Free-Energy **Tensor Compression**
- **Multicomponent** PF simulations
- Real-time surrogate predictions

Approach: Physics to Surrogate Pipeline

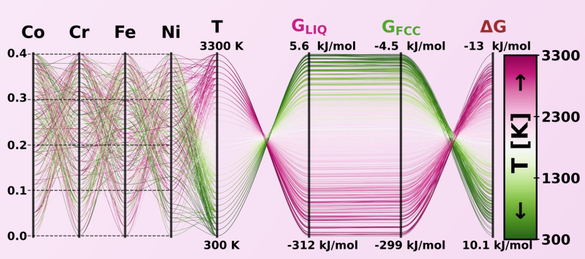
CALPHAD ⇨ Thermodynamic Data ⇨ Tensor Computation ⇩

Digital Twin ⇦ Attention Surrogate ⇦ Phase Field Dataset

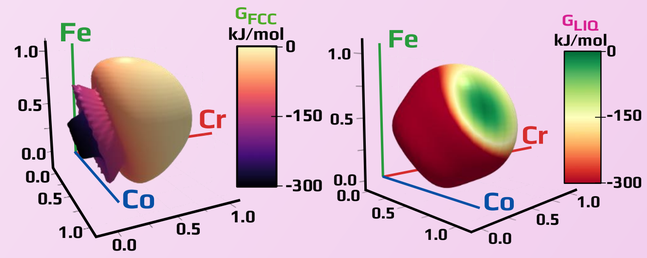
Methodology

CALPHAD Thermodynamic Tensor

Co-Cr-Fe-Ni Gibbs Free Energies



FCC and LIQUID phases

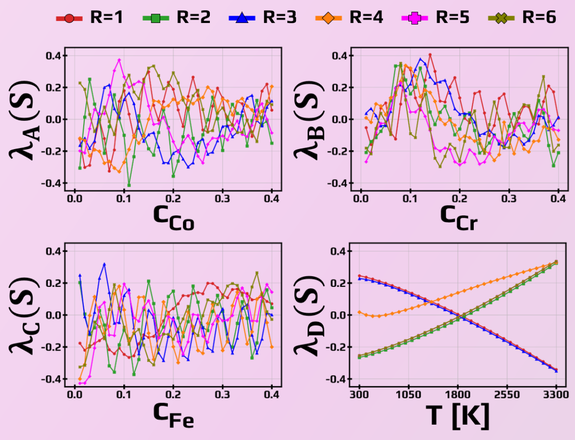


Tensor Computation

Canonical Polyadic Decomposition (**CPD**)

$$G_{c,T}^{CPD} \approx \sum_{r=1}^{R} \lambda_r A_r \otimes B_r \otimes C_r \otimes D_r$$

- Rank-structured TDT factorization *[1]*
- c-T mode loading vectors
- Smooth Quadratic $\boldsymbol{T}$ trends
- Oscillatory $\boldsymbol{c}$ response

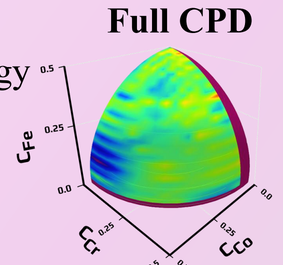


Quadratic Free-Energy Distillation

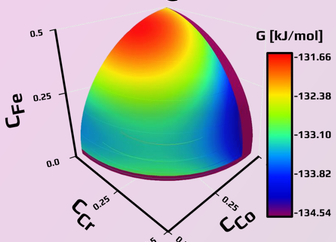
$$G_{c,T}^{Quad} = G_{eq} + \sum_{\alpha} A_{\alpha}\left(c_{\alpha} - c_{\alpha,eq}\right)^2 + A_T\left(T - T_{ref}\right)^2$$

- Compact analytical Free-Energy
- Quadratic in (**c,T**)
- Capture FCC/LIQUID
- PF ready thermodynamics

Full CPD

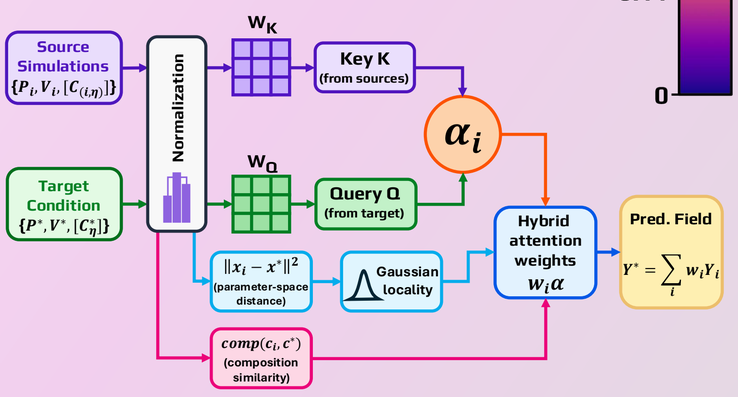


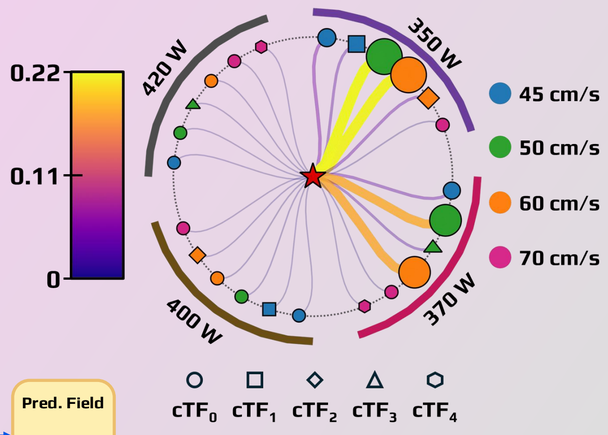
Full QUAD



Surrogate Model: Attention Based DT

- PF simulation: Knowledge Base
- Target State Space Vector as Query
- Attention weight: Nearest case
- Predicts **T, η** in real time

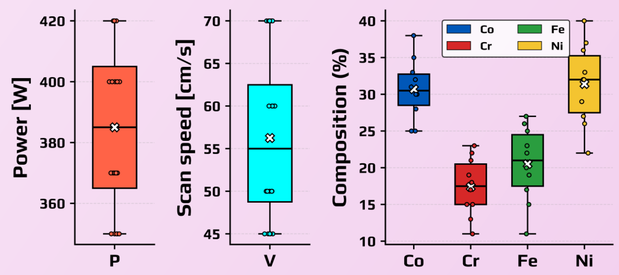




Target: 358W, 55cm/s

Results

Multiphysics Simulations



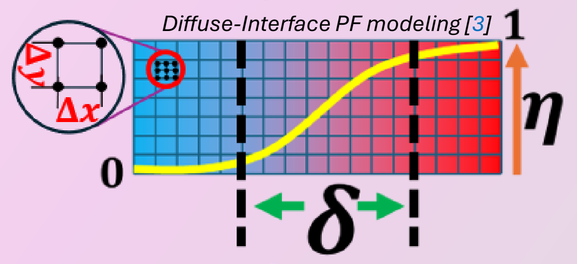
Laser-processing [2] & Composition Range

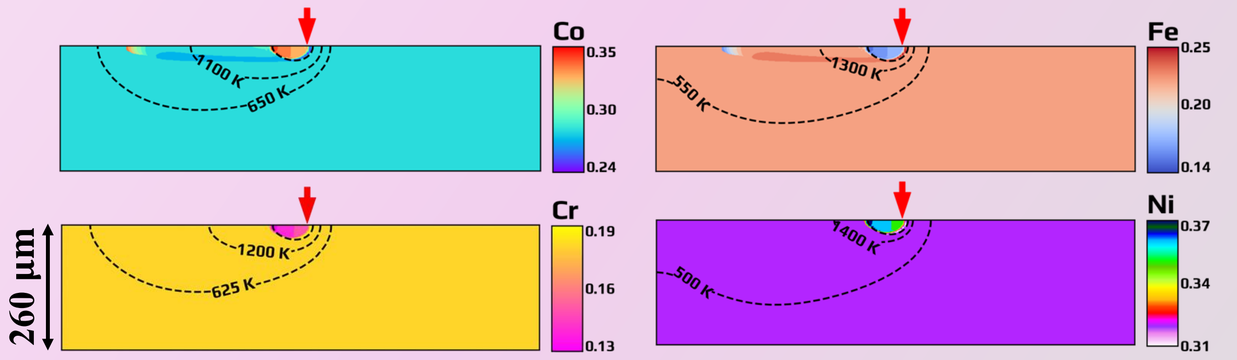
MOOSE

Heat Transfer, Phase-Field, Fluid Flow

PF O/P: **T** η_{LIQ} η_{FCC} c_{Co} c_{Cr} c_{Fe}

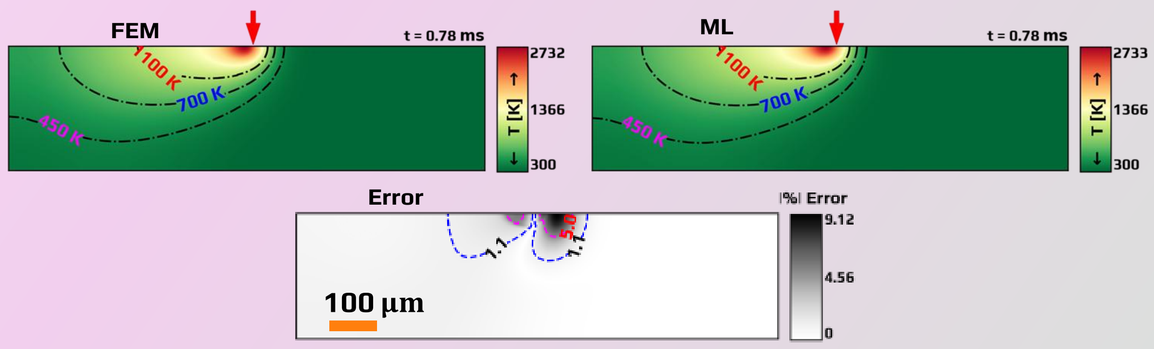
Diffuse-Interface PF modeling [3]





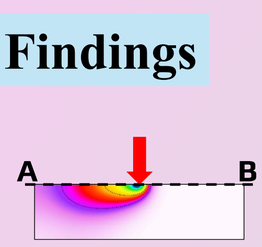
Elemental distribution maps @ 370 W, 50 cm/s

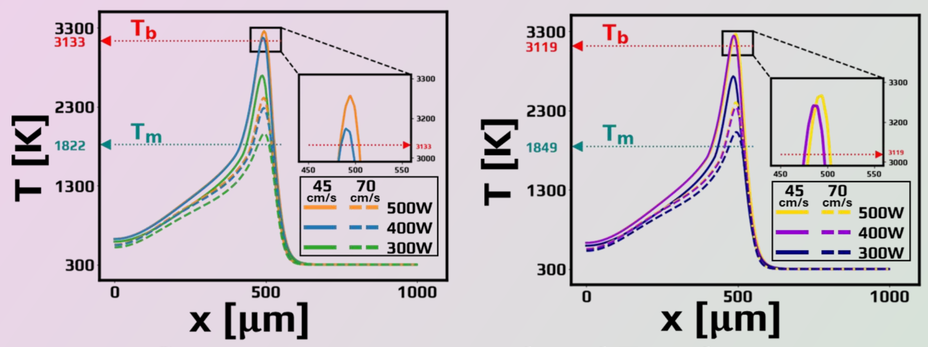
Model Predictions



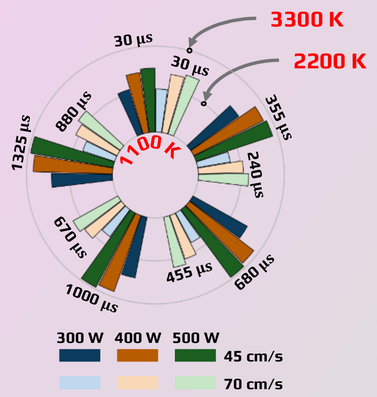
FEM vs AI surrogate model comparison with error analysis

Findings

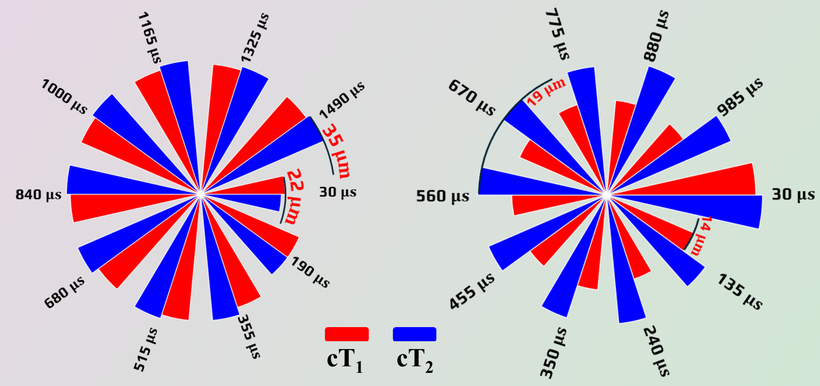




Composition-sensitive meltpool T prediction



Temporal peak-temperature response histogram



Predicted meltpool depth at 45 and 70 cm/s

References

[1] YA. Coutinho et at., *Combining thermodynamics with tensor completion techniques to enable multi-component microstructure prediction*, npj Computational Materials 6 (2020)

[2] S. Wang et al., *Superior strength-ductility synergy in additively manufactured CoCrFeNi high-entropy alloys with multi-scale hierarchical microstructure,* Journal of Alloys and Compounds 1006 (2024)

[3] N. Moelans et al., *An introduction to phase-field modeling of microstructure evolution*, Calphad 32 (2008)

Acknowledgements

NATIONAL SCIENCE CENTRE POLAND *UMO-2021/42/E/ST5/00339* *UMO-2023/51/I/ST11/02716*

fwo *G000225N*

Contact

upadesh.subedi@polsl.pl

https://subediupadesh.github.io