Computational Materials Science Laboratory

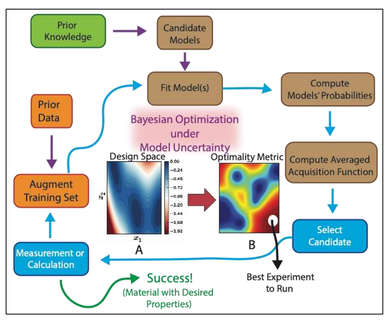
MATERIALS SCIENCE & ENGINEERING
TEXAS A&M UNIVERSITY

Dr. Raymundo Arroyave

Kubra Karayagiz, Luke Johnson, Thien Duong, Vahid Attari, Pejman Honarmandi, Tanner Kirk , Woongrak Son, Anjana Talapatra, Yuhao Wang

Materials Discovery: Efficient Global Optimization

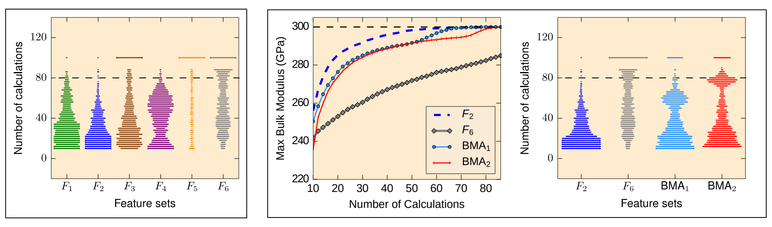
A platform for autonomous materials discovery



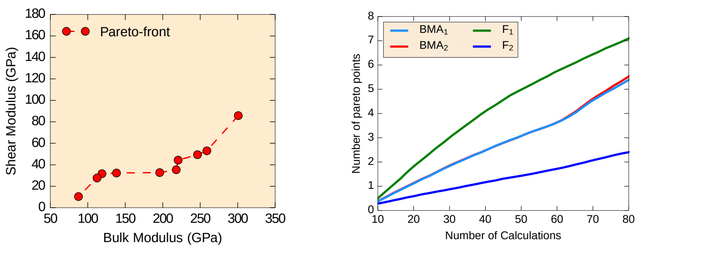
- For the class of 211/312 MAX phases Identify the MAX phase with
  - Maximum bulk modulus(K)
  - Minimum shear modulus(G)
  - Pareto front of materials with max K and min G
- Features used:
  - Electronic structure properties
  - Chemical composition
  - Empirical model parameters

Single Objective : Maximize Bulk Modulus

Bayesian Model Averaging (BMA)

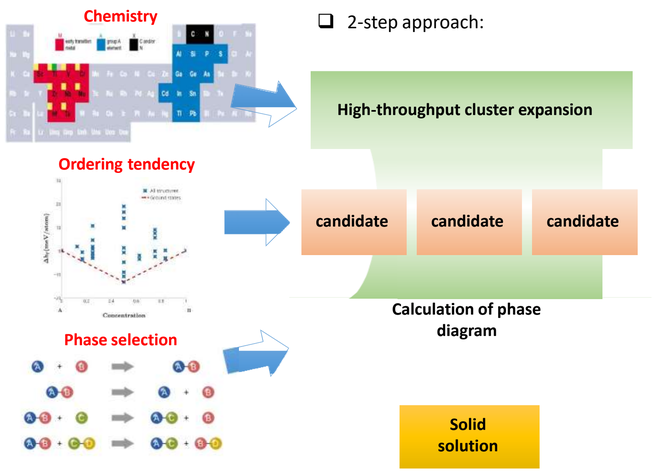


Multi-objective : EHVI – Maximize ductility index by maximizing K and minimizing G: table and bar chart representation of same data

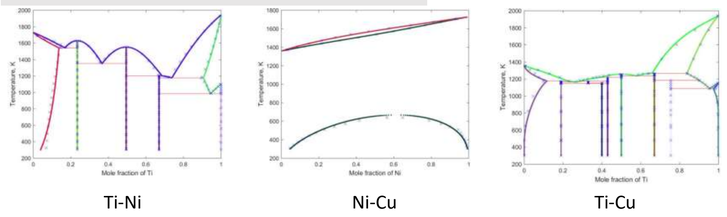


XichLo - A Material Design Studio

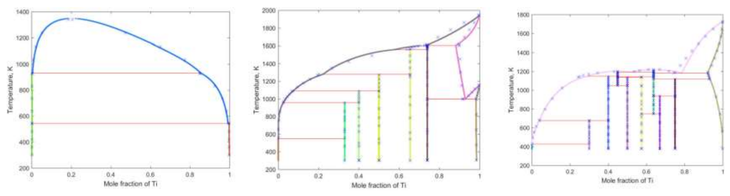
Motivation: Calculations of Ti2AlC – Cr2AlC phase diagram



Binaries

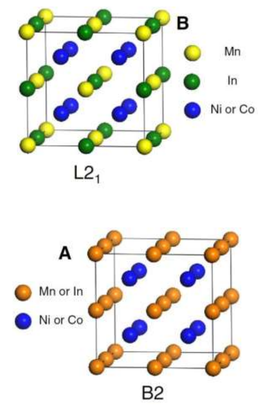


→ Established but there still room to expand

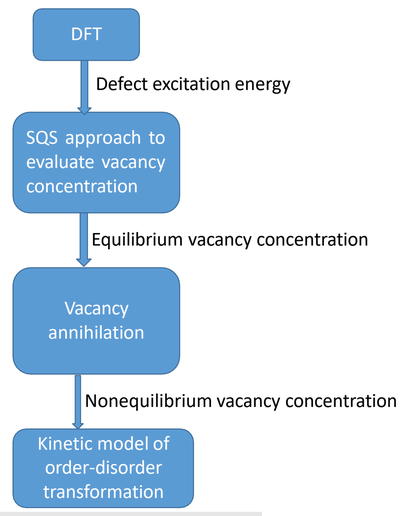


kinetics of B2–L21 Ordering in Ni-Co-Mn-In

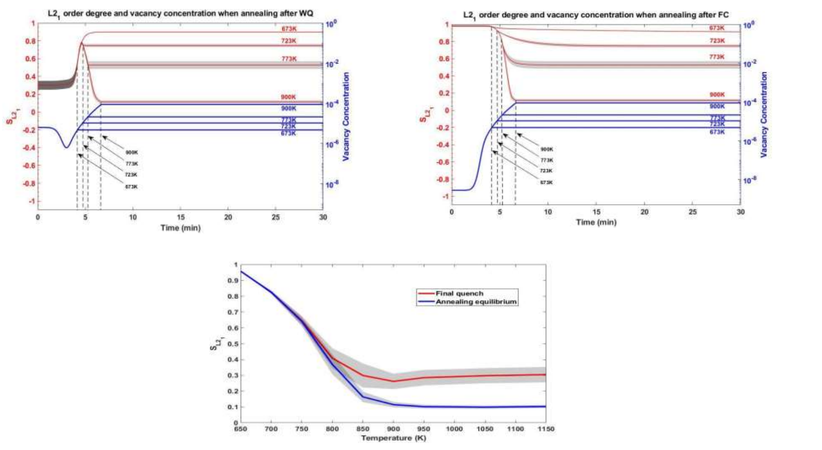
Order Disorder transformation



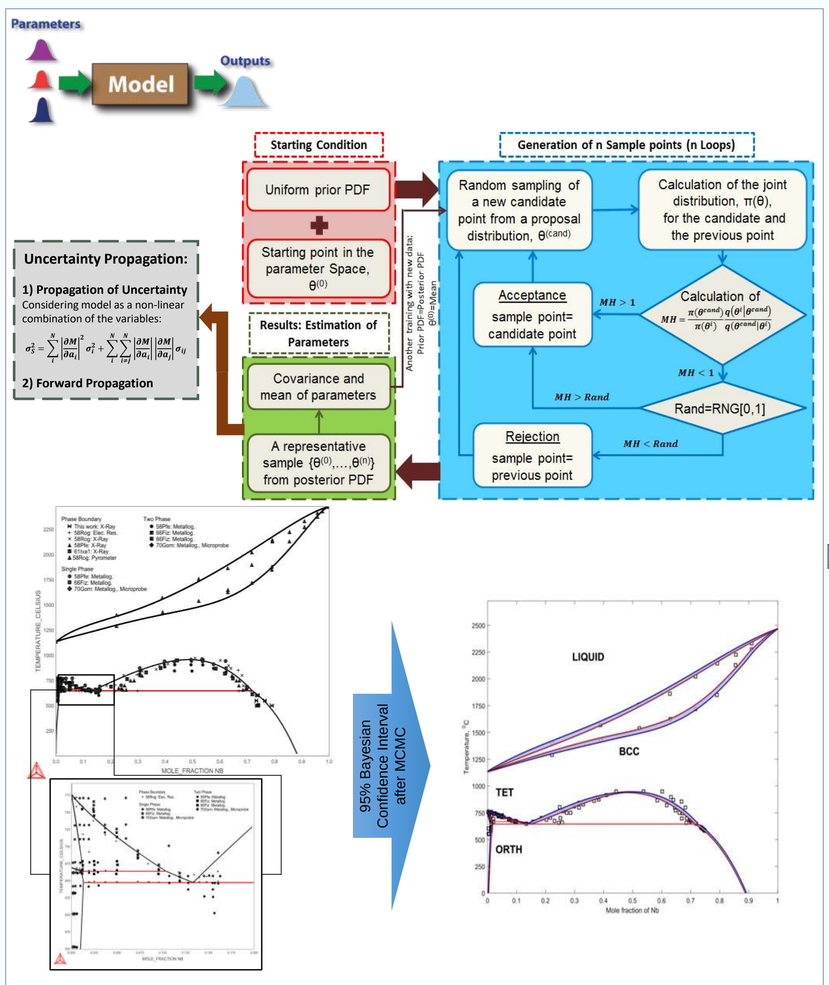
Model approach



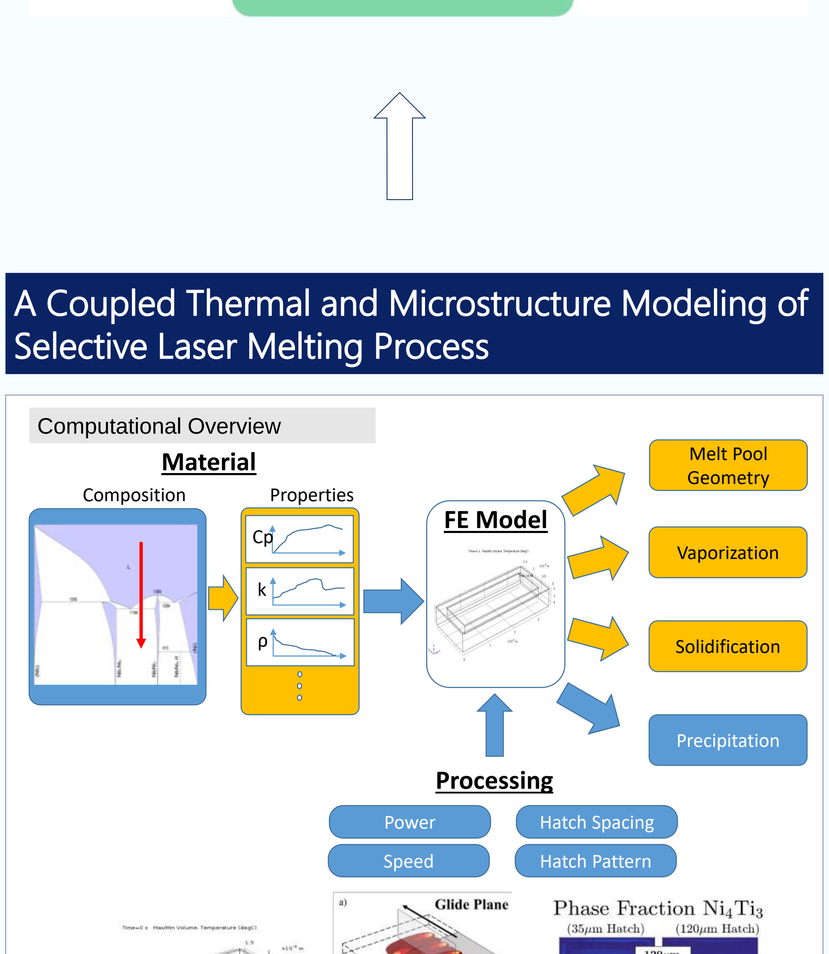
Calculated $L2_1$ order during annealing and final quenching



Design under Uncertainty Quantification

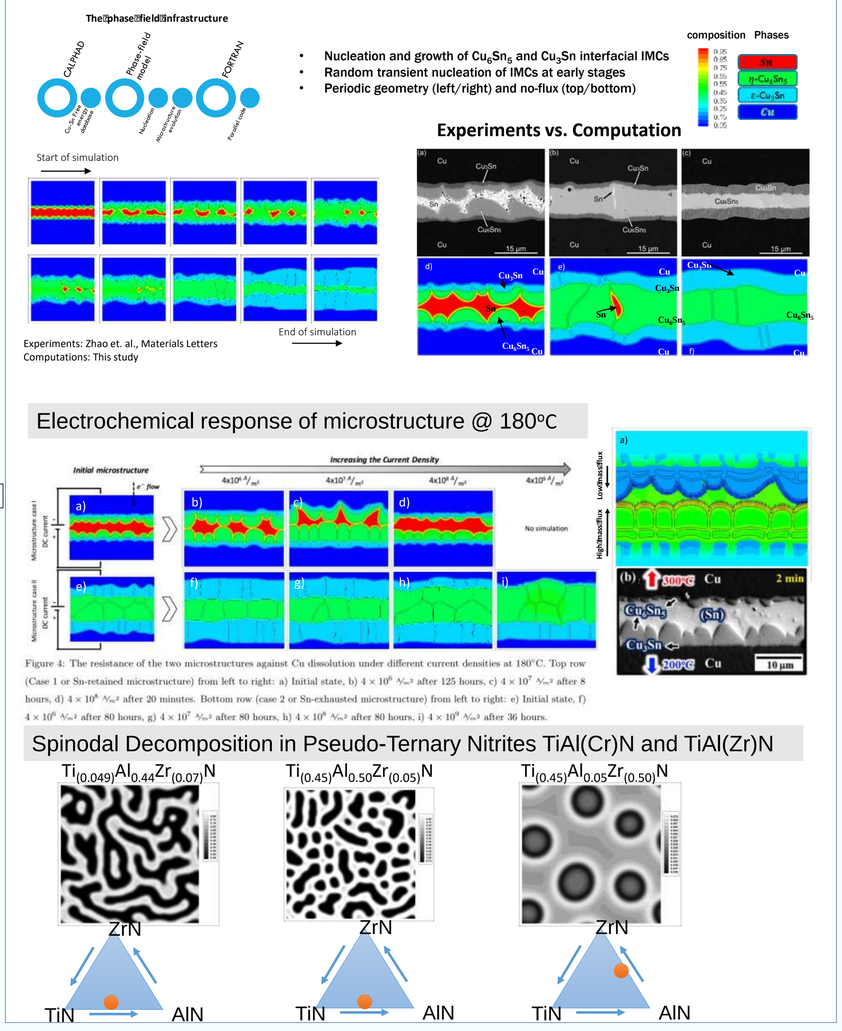


Thermo-Calc Optimized Phase Diagrams vs. MCMC Optimized Phase Diagram with Uncertainty Band



Phase Field Modeling: Electronic Materials

Microstructure Generation



A Path Planning Algorithm for Functionally Graded Materials Design

Problem Motivation

Functionally-Graded Material (FGM)
- Characterized by a variation in composition or structure gradually over volume

Consider an FGM made via Additive Manufacturing
- Composition changed layer by layer

[1]

Rapidly-Exploring Random Tree

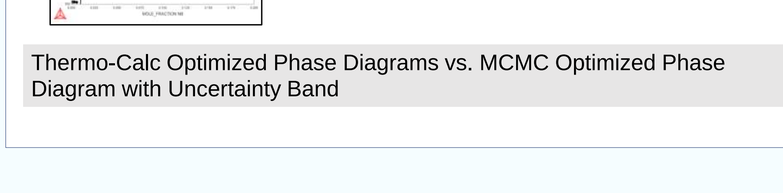
RRT*
Finds shortest path (optimal solution)

RRT*FN
Finds shortest path with less samples

[2]

Path planned successfully in FeNiCr space

No consideration of phases during cooling
Constraint: No sigma phase composition above 1%

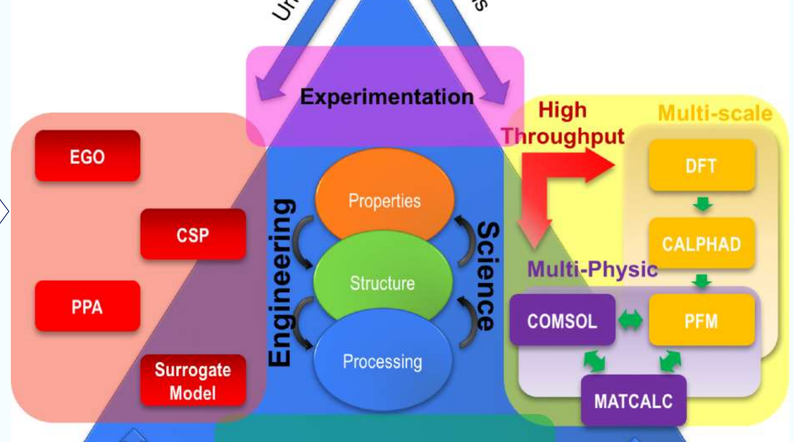


[1] Hofmann, Douglas C., et al. "Developing gradient metal alloys through radial deposition additive manufacturing." Scientific reports 4 (2014): 5357.

[2] Olzhas Adiyatov and Huseyin Atakan Varol. *Rapidly-exploring random tree based memory efficient motion planning*. In Mechatronics and Automation (ICMA), 2013 IEEE International Conference on, pages 354–359, 2013. DOI: http://dx.doi.org/10.1109/ICMA.2013.6617944

A Coupled Thermal and Microstructure Modeling of Selective Laser Melting Process

Computational Overview



Precipitation (NiTi)

Multi-Scale Multi-Physics Modeling of Inconel 718 during Selective Laser Melting

Overview of the Developed Modeling Framework

Investigation of the Effect of Kinetic Parameters on Growth Morphology