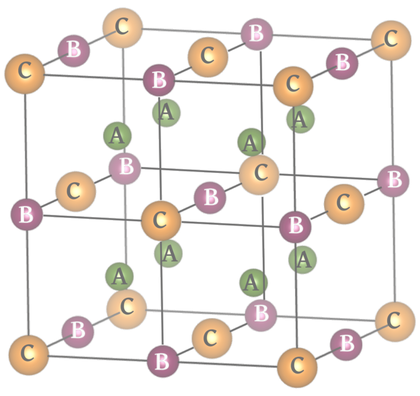
SUPERCOMPUTING @ COMPUTATIONAL MATERIALS SCIENCE LABORATORY

Materials Science & Engineering Department
Texas A&M University



TEXAS A&M UNIVERSITY

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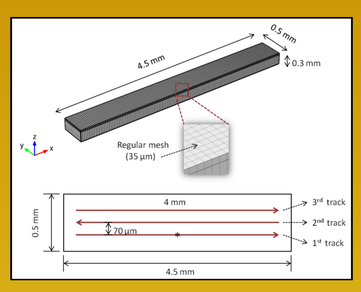
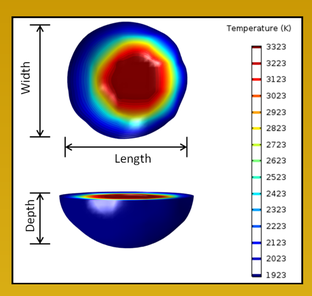
Selective Laser Melting

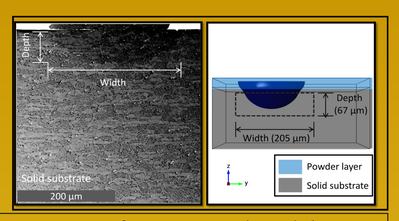
A 3D FE model was used to study the thermal behavior during selective laser melting (SLM) of Ti_6Al_4V through the use of Comsol Multiphysics software



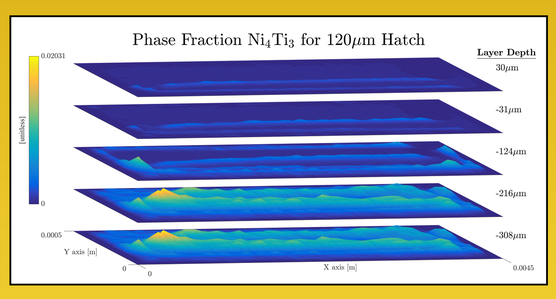
A 3D model consisting of a thin layer of powder and a thick substrate

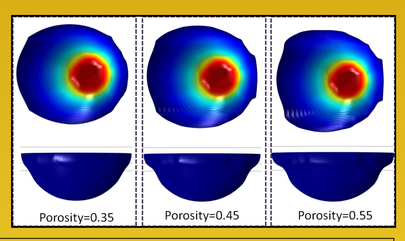


Melt pool size and geometry



Comparison of HAZ size in the solid substrate from exp *(left)* and simulation *(right)*



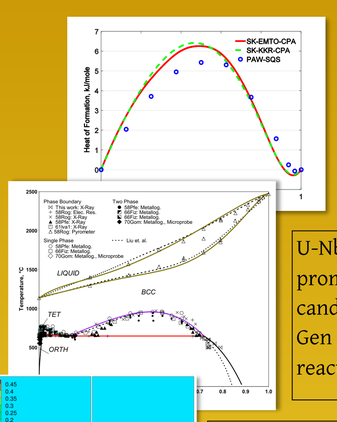


Change in the predicted HAZ geometry and size for different porosity values

Clusters Used: Ada
Softwares Used: COMSOL, MatCalc
Typical Job Size: 20 Cores, 240 MB, 168 hrs

Phase Field

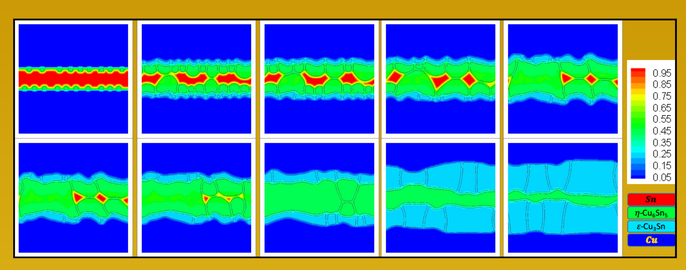
Thermodynamics & Kinetics of the U-Nb fuel system



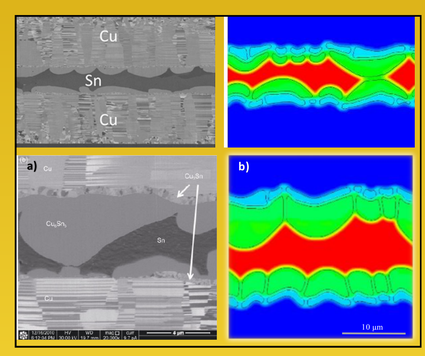
U-Nb is a promising fuel candidate for Gen IV nuclear reactors

The discontinuous precipitation (or cellular reaction) of U-Nb has been demonstrated and shows reasonable agreement with experiment across length

Phase Field Modeling of Joint Formation During Isothermal Solidification in 3DIC Micro Packaging



Evolution of the microstructure during isothermal reflow process at T = 250 °C for the interlayer thickness of 5 µm



Comparing the exp observations with the computational results. a) FIB cross-sectional image of a microjoint formed with Cu substrates and Sn interlayer. b) The computational result for reflowing at 250 °C with initial interlayer thickness of 10 µm

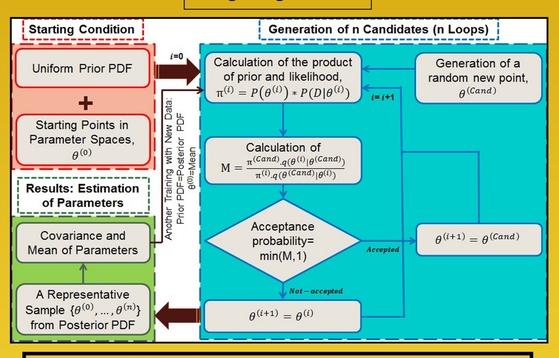
Clusters Used: Ada
Softwares Used: Fortran (inhouse), VASP
Typical Job Size: 96 Cores, 300 MB, 96 hrs

Alloy Design Using Bayesian Approaches

TRIP Steel Design by:

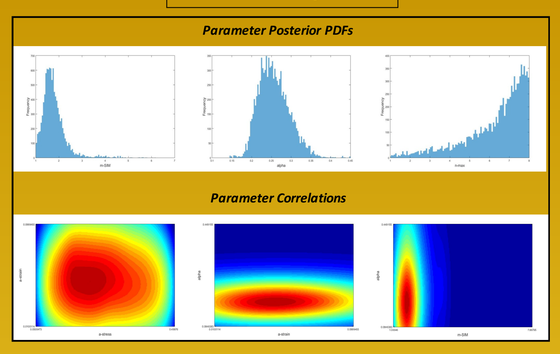
- Introduction of a physically-based model for predicting the plastic flow behavior in order to reduce the experimental cost
- Modelling complexities associated with the contribution of several constituent phases and strain-induced martensitic transformation (SIMT) during plastic deformation
- Model Parameter Calibration Using Bayesian method based on Metropolis-Hastings Markov Chain Monte Carlo (MCMC) algorithm

Design Algorithm

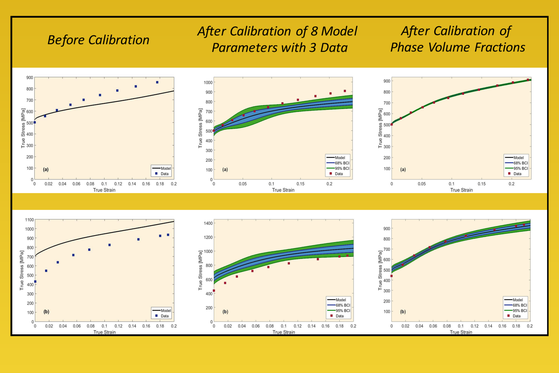


Clusters Used: Ada
Softwares Used: Fortran (inhouse)
Typical Job Size: 20 Cores,240 MB, 336 hrs

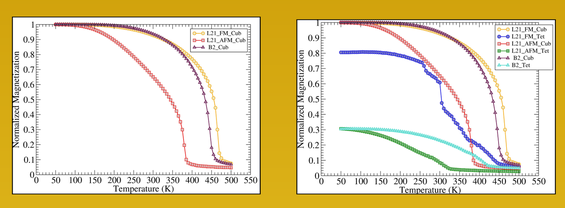
Parameter Analysis



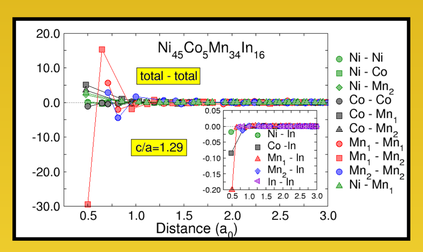
Comparison of Model Results and Experimental Data
(2 Examples from Jacques 2001)



- q-state Pott's model is used to take into account the discrete magnetic states of magnetic atoms
- The glass system is characterized by the presence of field-cooling (FC) and zero-field cooling (ZFC) curves
- The total interaction between spins is defined using the Heisenberg Hamiltonian

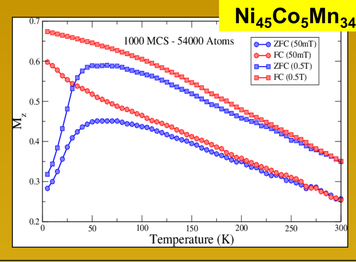


Normalized Magnetization as a function of Temperature (K). Due to the presence of large AFM interactions in martensite, the classical Heisenberg's model is more suited for these studies

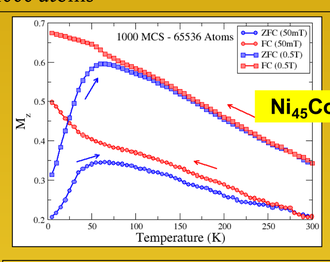


Exchange interactions

$Ni_{45}Co_5Mn_{34}In_{16}$



ZFC and FC curves for $Ni_{45}Co_5Mn_{34}In_{16}$ alloy calculated using the Heisenberg model using 54000 atoms



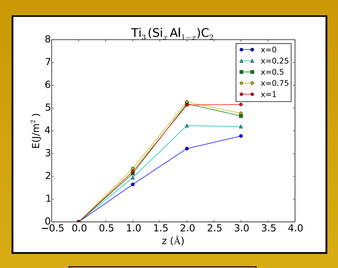
ZFC and FC curves calculated using the Heisenberg model using 66536 atoms

Clusters Used: Ada, Lonestar, Lonestar5
Softwares Used: Tammal (inhouse), VASP, EMTO-CPA, SPR-KKR, Python, Matlab
Typical Job Size: 20 Cores, 512 MB, 168 hrs

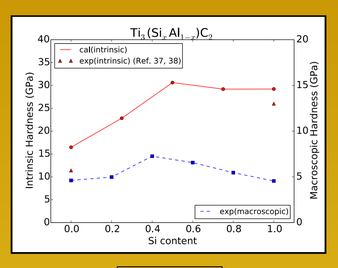
Strain glass modeling using Monte-Carlo techniques

High Throughput Materials Design

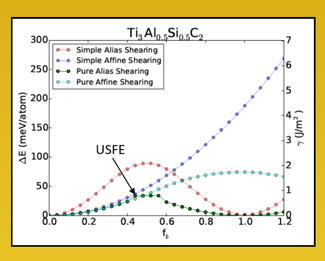
Mechanical Properties of $Ti_3(Al,Si)AlC_2$



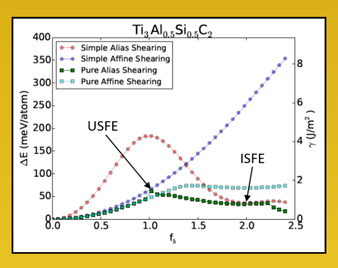
Cleavage energy



Hardness



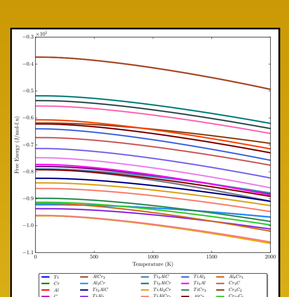
under <0110> {0001} shear



under <2110> {0001} shear

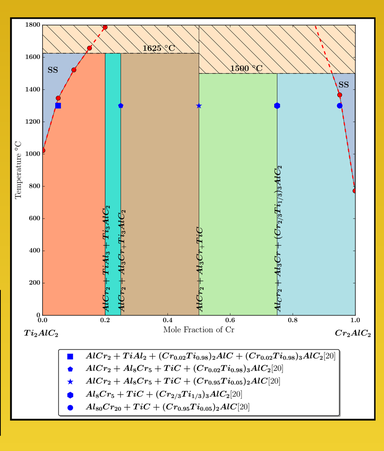
Energy as a function of fraction of Burgers vector f_b

Finite-temperature phase stability of $(Ti,Cr)_2AlC$



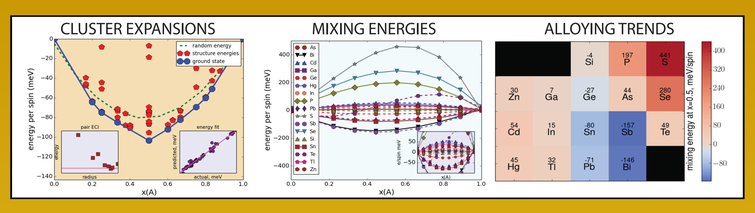
The vibrational and electronic contributions to the total energies of the system to better approximate finite-temperature free energy of the system were accounted for using first-principles calculations within the framework of DFT

Phase competition between $(Ti,Cr)_2AlC$ alloys with other quaternary, ternary, binary, and unary systems were considered via energy minimization subjected to mass-conservation constraint.



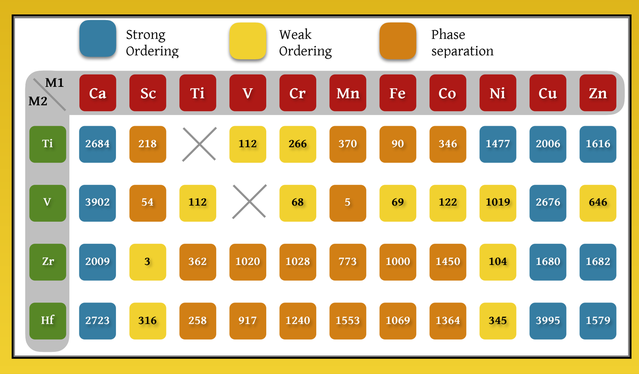
Clusters Used: Ada, Lonestar, Lonestar5
Softwares Used: Tammal (inhouse), VASP, EMTO-CPA, SPR-KKR, Python
Typical Job Size: 96 Cores, MB, 240 MB, 96 hrs

Solid solution alloying characteristics using cluster expansions in MAX phases



- The possibility of alloying MAX compounds not only enables finer tuning of their properties but can also be used to stabilize compounds that may otherwise be metastable in their pure state.
- An ab initio-based investigation of the intrinsic alloying behavior in the A sub lattice is carried out to identify alloying trends

Mixing in M lattice



This work was carried out by Kubra Karayagiz, Luke Johnson, Thien Duong, Vahid Attari, Pejman Honarmandi, Navdeep Singh, Woongrak Son, Anjana Talapatra and Raymundo Arroyave with support from NSF, AFOSR, AFRL, NASA, DOE, and LLNL. For additional information, please refer: https://sites.google.com/a/arroyavelab.net/wiki/