High entropy alloys for beam windows: simulation, pre-characterization, and ion irradiation

Gaurav Arora

TSD Topical meeting

Feb 2024

Introduction

Major accelerator facilities have had to limit their beam powers because of the survivability of their targets and windows, rather than as a limitation of the accelerators themselves

More power → More challenges

- More radiation damage
- Increased thermal shock and thermal fatigue

Ammigan, Kavin, and Frederique Pellemoine.FERMILAB-CONF-22-107-AD. Fermi National Accelerator Lab.(FNAL), Batavia, IL (United States), 2022.

Radiation damage, Thermal shock and Fatigue

Radiation damage

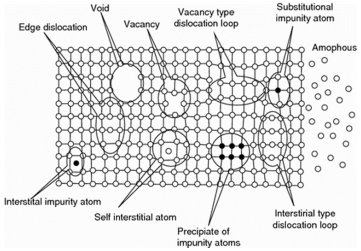
Atomic Displacements: Radiation can cause atoms within a material to be displaced from their original positions, leading to structural defects.

Crystal Lattice Damage: The displacement of atoms can disrupt the crystal lattice structure of a material, affecting its mechanical properties.

Microstructural Changes: Radiation can induce changes in the material's microstructure, such as the formation of dislocation loops and voids.

Embrittlement: Radiation damage can make materials more brittle, reducing their toughness and resistance to fracture.

Swelling: Radiation-induced defects can lead to volumetric swelling, which can have implications for material stability.



D.L. Porter and F. A. Garner, J. Nuclear Materials, **159**, p. 114 (1988)

Thermal shock

Stress and Strain: The abrupt temperature change creates stress and strain within the material, as different parts expand or contract at different rates.

Example: 1 MW target: ~250 K in 10 μs pulse (2.5 x 10^7 K/s)

Cracking and Damage: Thermal shock can lead to cracking, fracture, or other forms of damage in the material.

Fatigue

Abrupt changes in temperature causes fatigue leading to reduced life, crack propagation, and decreased toughness.

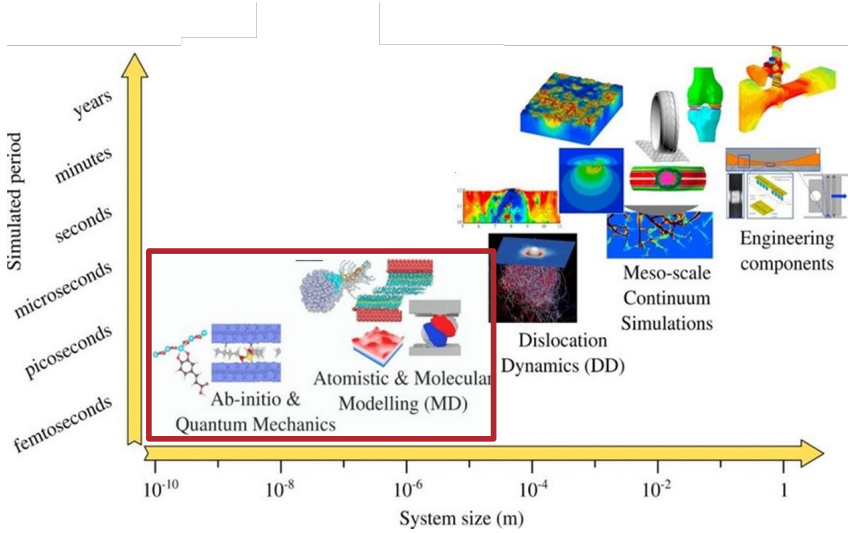
Overarching goal

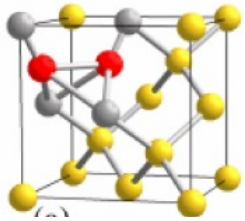
Develop materials capable of withstanding higher levels of beam power for extended operational lifespans

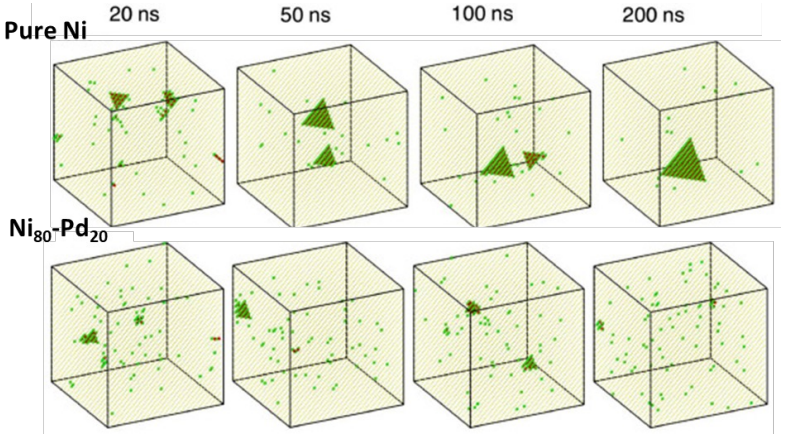
How to achieve?

Using simulation techniques along with experiment for developing new materials

Types of simulations: Time *vs.* system size







- Density functional theory (DFT): Defect formation energies, band gap, etc.
- Molecular dynamics (MD): Radiation damage such as void formation, evolution of system with respect to temperature, etc.

Goel, Saurav, et al. Materials Today Chemistry 18 (2020): 100356
Arora, Gaurav, et al." Materialia 15 (2021): 100974

Overview of density functional theory (DFT)

Basic definition

- DFT is a quantum mechanical modeling method used to study the electronic structure and properties of materials.
- It provides insights into the behavior of atoms and molecules at the atomic scale.

Advantage of DFT

- Wide applicability: DFT can be applied to range of materials to study electronic structures, charge density, magnetic and more.
- Does not require any input from the experiment as it uses fundamental equations to solve the problem
- Insight into chemical and physical processes: Offers deep understanding of the chemical reactions, electronic transitions and physical phenomena at atomic level.
- Complement experimental results.
    - Allows the extraction of additional information such as atomic structures, reaction pathways.

DFT serves as powerful tool for screening and analyzing electronic properties of the materials before they are even synthesized

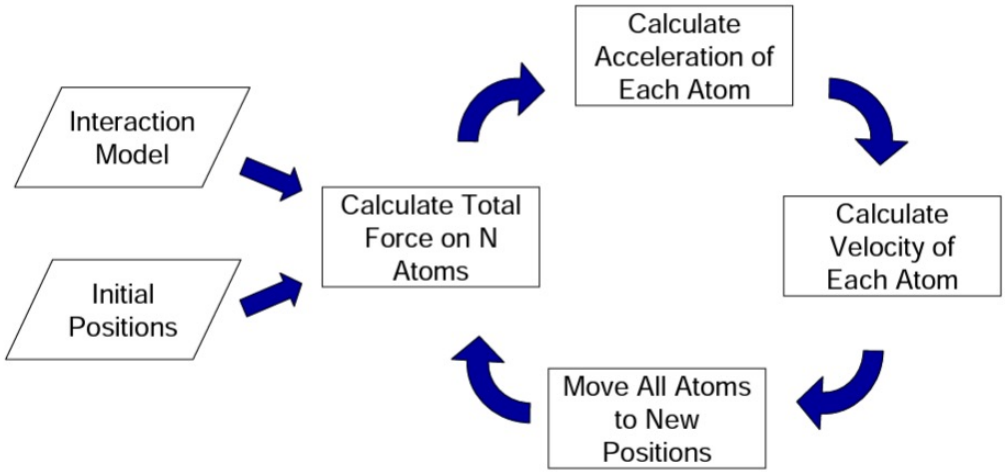
Overview of molecular dynamic (MD)

Basic definition

- Based on classical physics and is used to describe positions, velocities, and orientations of molecules over time.
- Energy/forces are calculated using Newton's law of motion.

Advantages

- System can be simulated using different conditions, for example at very high temperature and pressure.
- Visualize the evolution of system with time.
- Millions of atoms can be modeled.



MD serves as powerful tool for studying microscopic properties of materials

https://www.compchems.com/molecular-dynamics-md/#advantages-and-disadvantages
https://nanohub.org/resources/7573/download/Martini_L1_Introduction.pdf

Fermilab

Summary of DFT and MD

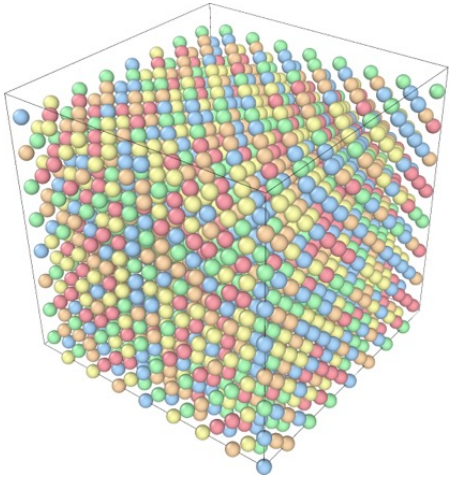
DFT	MD
• Work on the principle of quantum physics	• Work on the principle of Newton laws
• Highly accurate	• As accurate as interatomic potentials
• Computationally expensive	• Computationally cheap
• Limited to ~300 atoms	• Million of atoms can be modeled
• Software: VASP, Q-espresso, etc.	• Software: LAMMPS

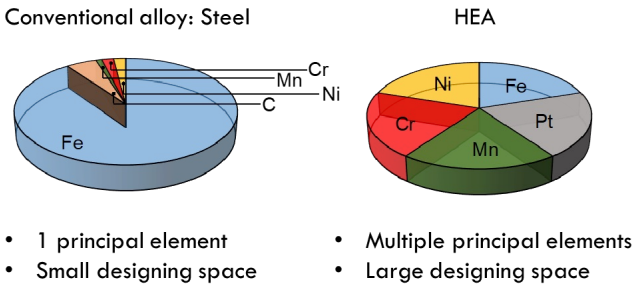
Interatomic potentials

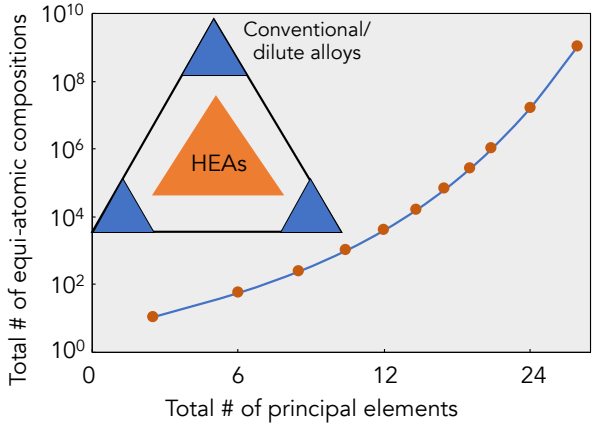
- Mathematical function for calculating potential energy of the system with given positions of atoms.
- Equations are fitted using data derived from DFT and/or experiments.
- Not all the properties can be derived from just one form of inter-atomic potentials.
- Accuracy of the simulations depends upon the accuracy of the interatomic potentials.

Development of accurate interatomic potentials is the key challenge in designing or studying defect properties of materials

Overview of high entropy alloys (HEAs)







- Multi-principal elemental alloys
- Random solid solution
- Equi-atomic or near equi-atomic composition
- FCC, BCC or HCP crystal structures
- Distorted lattice

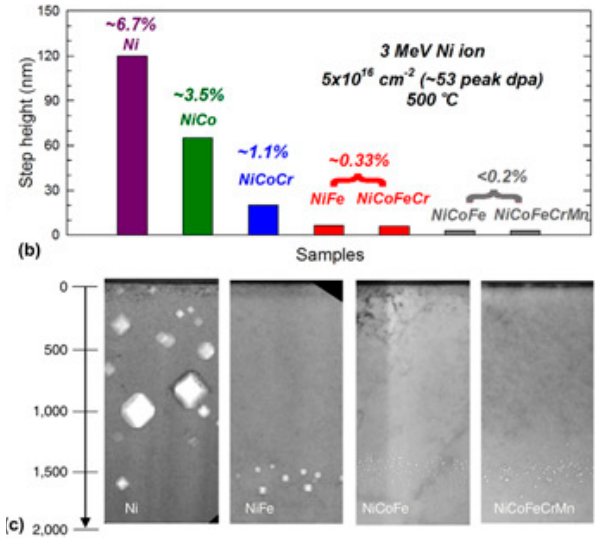
- Large number of HEAs can be designed by changing the chemistry and composition of principal elements.
- Simulations provide an opportunity for exploration.

Yang, Tengfei, et al.Journal of Materials Research 33.19 (2018): 3077-3091.

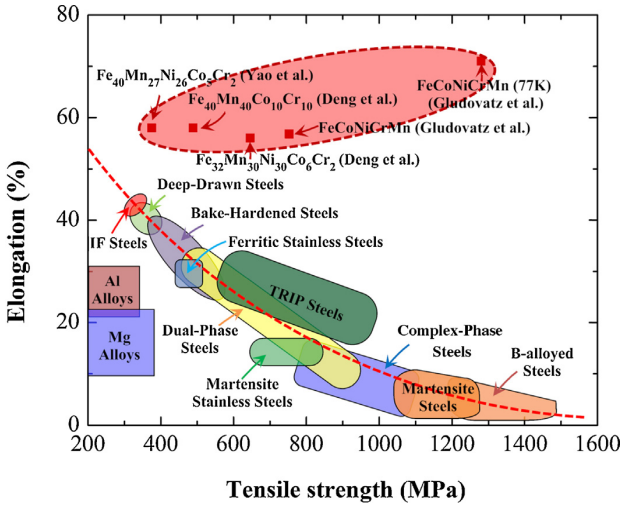
Fermilab

Exceptional properties of High entropy alloys (HEAs)

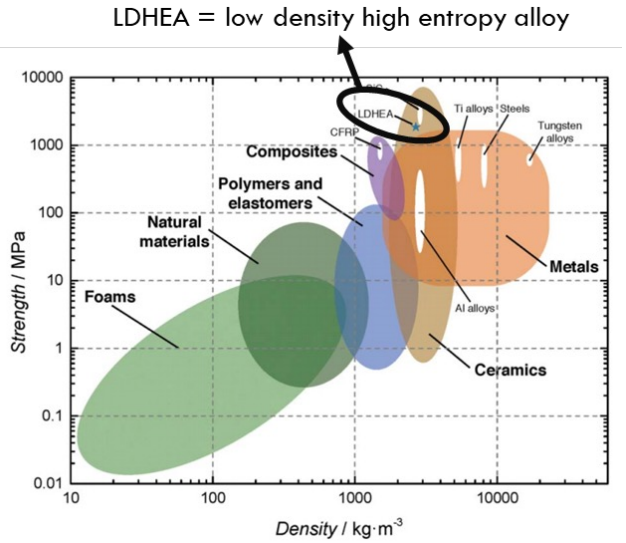
Radiation tolerant property of HEAs



High strength along with high ductility



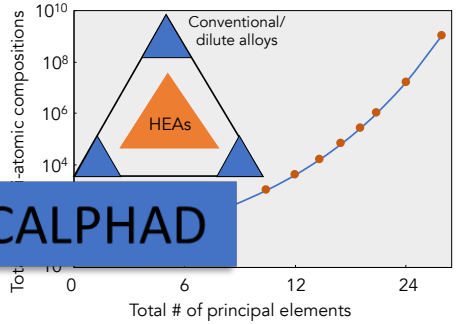
High strength while maintaining low density



HEAs offer a new route for exploring and designing next generation material for beam windows

Oh et al., Nat Comm. 10, 2090 (2019)
Youssef et al., Materials Research Letters, 95-99 (2015)
Jin et al., Scripta Materialia 119 (2016)

Design process for HEAs



Find suitable compositions from the large design space using CALPHAD

Single phase over large range of temperature

Perform density functional theory calculations

Strain calculations | Point defect calculations | Migration barriers calculations

Making of new inter-atomic potentials

Running MD simulations

- CALPHAD stands for "Calculation of Phase Diagrams."
- Used for making phase diagrams.

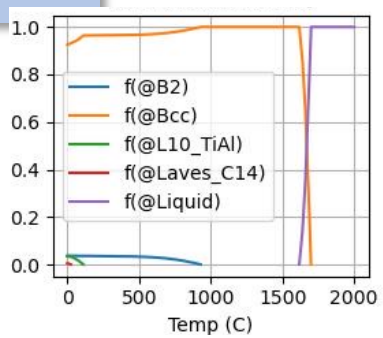
Fermilab

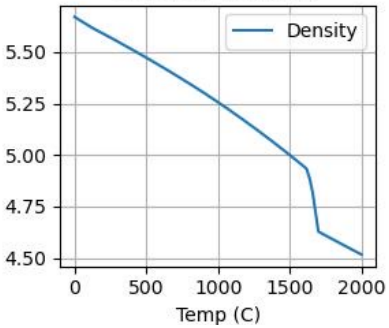
Exploring large design space using CALPHAD

Find suitable compositions from the large design space using CALPHAD

Single phase over large range of temperature

- Cr-Mn-V base ternary alloy to avoid high activation elements
  - Single phase BCC crystals
- Additional elements for improved strength
  - Ti as impurity getter
  - Al for lower density
  - Co to from semi-coherent B2 phase for strengthening





Range of elements explored (~120,000 combinations were explored)

	Al	Co	Ti	Cr	Mn	V
Min	0	0	0	0	0	0
Max	20	5	20	50	50	50
Step (at%)	2	1	2	3	3	Bal

Alloy compositions sorted by single-phase BCC/B2 temperature range

In collaboration with UM-Madison Materials Degradation under Corrosion and Radiation (MADCOR, Dr. Couet)

Fermilab

Selected HEAs for further exploration

1. Study the effect of Ti concentration
   - Al10-Co4-Cr25-Mn26-Ti1-V34
   - Al10-Co4-Cr27-Mn21-Ti4-V34

2. Study the effect of Co concentration
   - Al16-Co2-Cr25-Mn30-Ti1-V26
   - Al16-Co4-Cr25-Mn30-Ti1-V24

3. Study the effect of Al and removing Cr
   - Al20-Co1-Mn27-Ti2-V50
   - Al12-Co3-Cr6-Mn27-Ti2-V50

4. Study the effect of removing Co
   - Al18-Mn30-Ti2-V50
   - Al20-Co2-Mn26-Ti2-V50

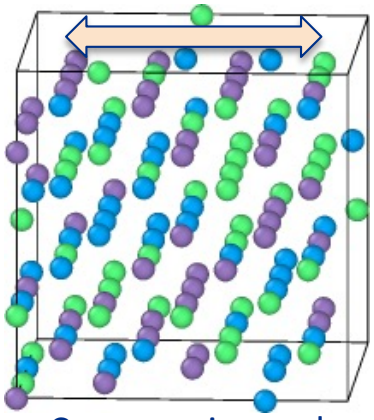
In collaboration with UM-Madison Materials Degradation under Corrosion and Radiation (MADCOR, Dr. Couet)

DFT simulations

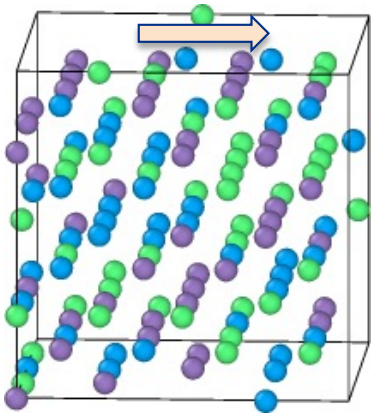
Perform density functional theory calculations

Strain calculations | Point defect calculations | Migration barriers calculations

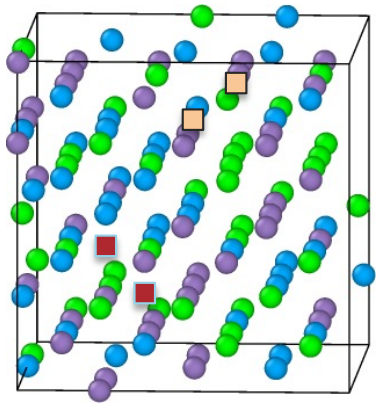
- To study the evolution of system following set of simulations are performed



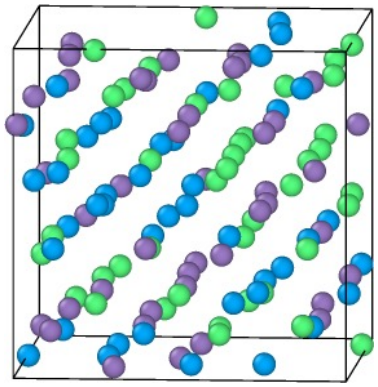
Compressive and tensile strain



Shear strain



Vacancies and interstitial



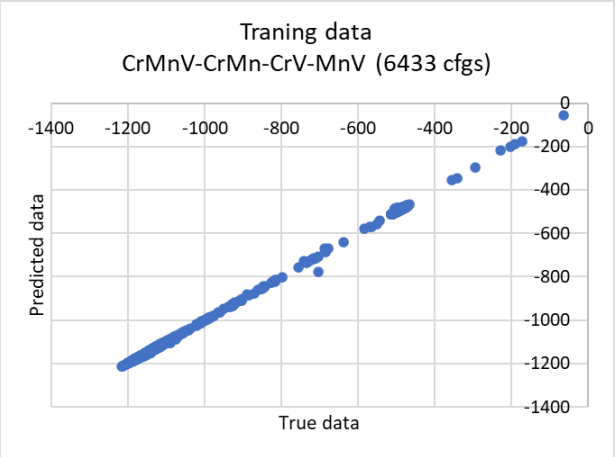
Different temperature

- Approximately 600 simulations are performed for each composition.
- Forces and energies are extracted and fed into making of machine learning potential.

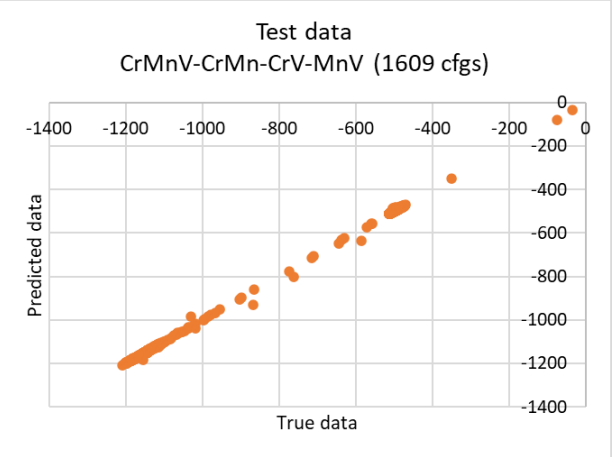
Fermilab

Preliminary results

- Data was trained for CrMnV equimolar and CrMn, CrV, and MnV binaries having different compositions. (~8000 simulations)



MAE (meV/atom): 14.33
Pearson: 0.99



MAE (meV/atom): 14.47
Pearson: 0.99

Model can predict energies accurately over a wide range

Conclusion and future work

- HEAs needs to be explored further for designing new alloys.
- Simulations could serve as powerful techniques for exploring the phase space.

Future work

- Analyze the results and find what kind of simulations/structures are contributing to higher errors.
- Run more DFT simulations and expand the dataset for training machine learning potentials and analyze the effect of different elements.
- Use trained model for predicting behavior of material under extreme conditions.

Acknowledgement

- HPT R&D group at Fermilab:
  - Frederique Pellemoine
  - Kavin Ammigan
  - Sujit Bidhar
  - Abraham Burleigh

- University of Wisconsin-Madison
  - Izabela Szlufarska
  - Dane Morgan
  - Adrien Couet
  - Nicholas Crnkovich

Thank you!