An Atomistic Study of the Radiation Resistance of Grain Boundaries in High Entropy Alloys

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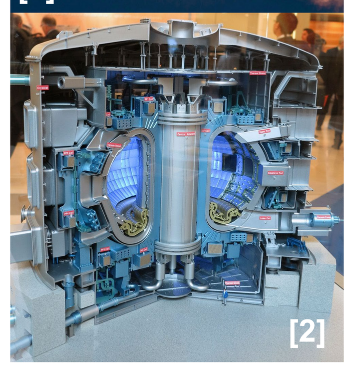
Introduction

A Radiation Resistant Material is Needed

- In nuclear systems, fusion reactors, space exploration, etc. materials are exposed to large fluxes of energetic atomic particles.
- These particles irradiate a material, causing radiation defects.
- These defects change the material properties.
- Need for a radiation resistant material that a can withstand mechanical extremes.



High Entropy Alloy's are a Strong Contender

High Entropy Alloys (HEA) Metallic alloys made of at least 5 elements in similar compositions.

Great for unique properties:
- High fracture toughness[3]
- Corrosion resistance[3]
- Extreme temperature[3]

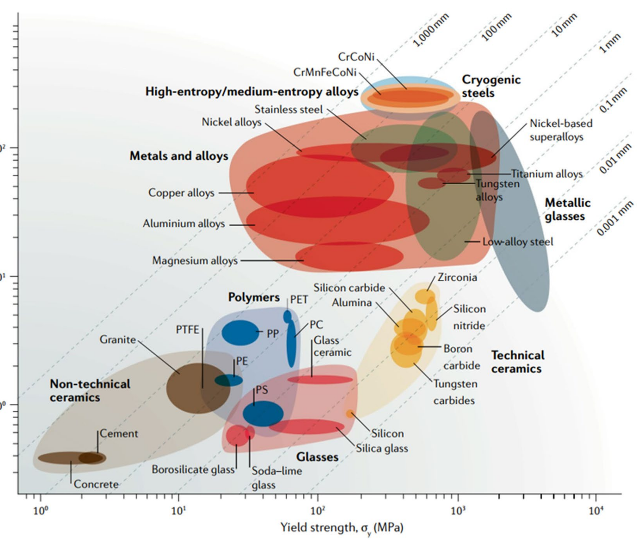
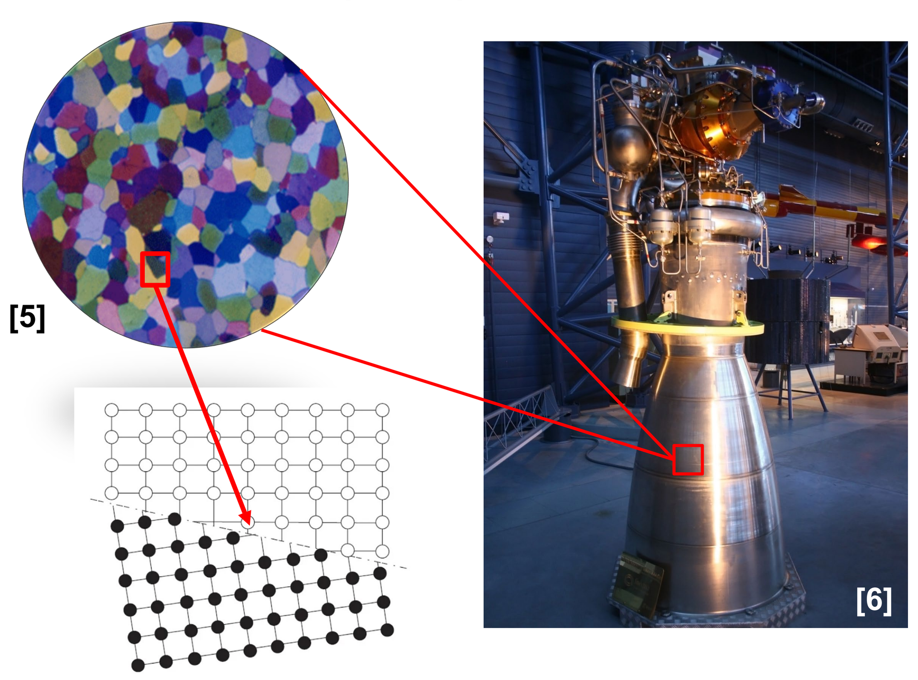


Figure 1. Ashby plot of strength versus fracture toughness [4]

Grain Boundaries and Radiation Damage

- Metallics like HEA's are polycrystals; they are composed crystalline grains that meet at internal interfaces termed **grain boundaries (GBs)**.



- GBs enhance a materials radiation tolerance by acting like a sink and absorbing the radiation induced damage.

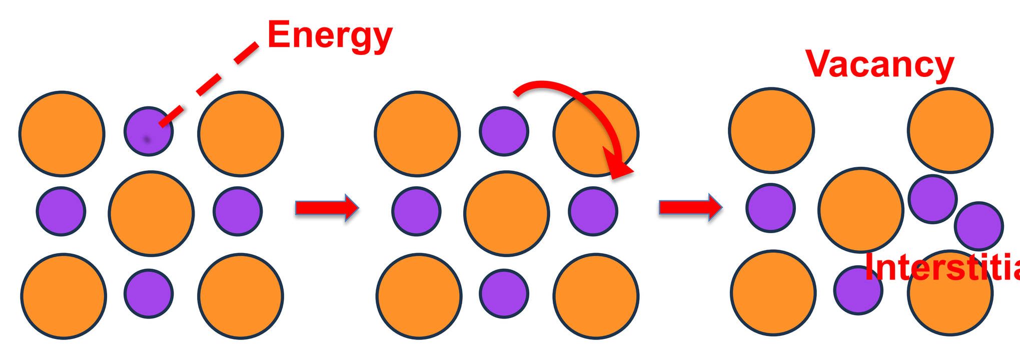
Hypothesis

GBs in HEAs reach steady state disordered structures under continuous radiation damage localized at the GB.

Methods

How a material is irradiated

- Energetic particles bombard a solid and atoms are displaced from their lattice sites.
- Creation of radiation damage or defects.
- The defect of focus are **Frenkel Pairs (FP)** which comprise of the interstitial and vacancies that result from irradiation.



Simulated Radiation

- To create FPs in an atomistic simulation we use a **Creation-Relaxation Algorithm (CRA):**
  1) Randomly select an atom and <u>displace</u> it with random direction and magnitude.
  2) Followed by a potential energy <u>minimization</u> to equilibrate the system.
  3) The process is <u>repeated</u> for a specified amount.

Material and Properties of Choice

- HEA: FeNiCrCoAl
- EAM Potential
- Sigma 17 Asymmetric GB
- MCMD Equilibrium
- Fixed volume conditions
- Temperature: 0 K

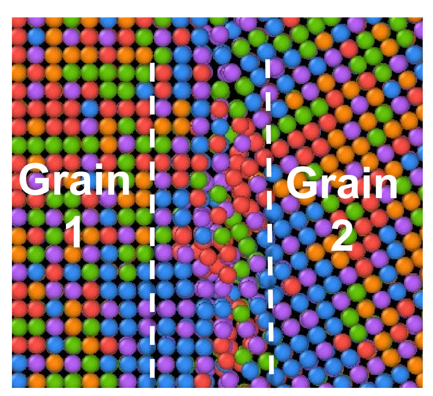


Figure 2. Grains and GB

CRA Specifications

- Radiation Zone Width: 10 Å
- Number of FP per step: 50
- Repeated for: 1000 steps

Results

Grain Boundary Changes

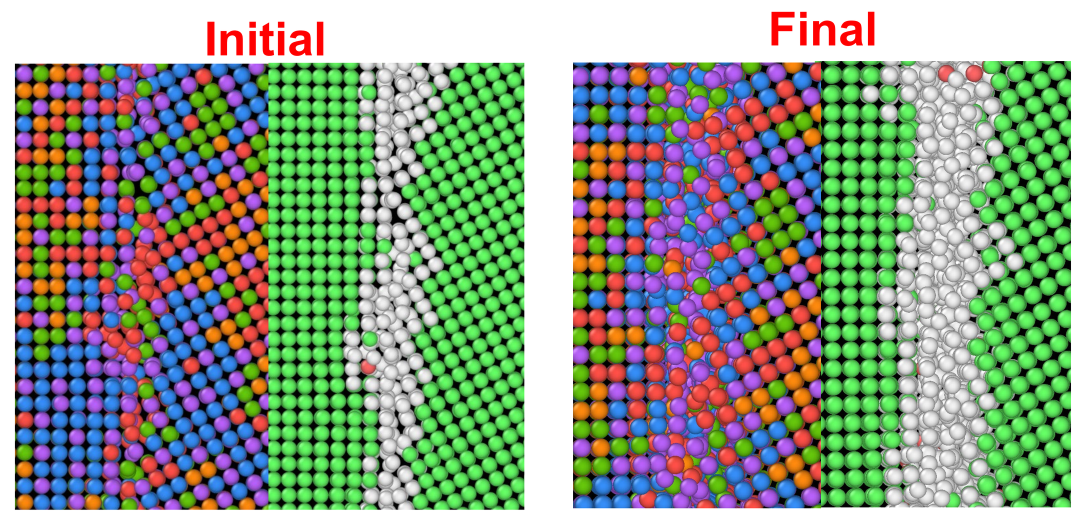


Figure 3. Structure before and after CRA comparison

Irradiation induced steady state microstructure

- To quantify the amount of irradiation, **DPA (Displacement per Atom)** is used.

$$DPA = \frac{\#\ of\ FP}{\#\ of\ Atoms\ in\ the\ Radiation\ Zone}$$

[6]

- The energy and the structure reach a saturated steady state.

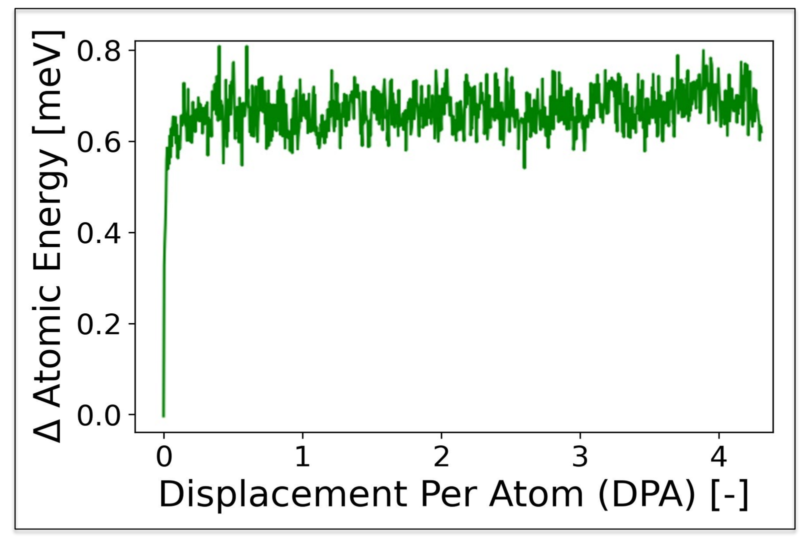


Figure 4. Change of Energy with irradiation

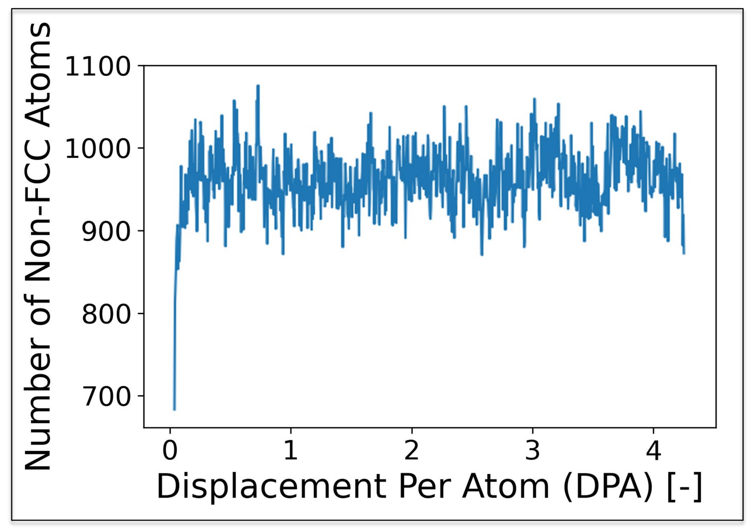


Figure 5. Change of GB Width with irradiation

- The GB width reflects structural convergence.
- The width is measured by the # of Non-FCC atoms
- Saturation of defect populations at and near the GB

Evolution of Concentration Profiles at the GB

- Radiation damage initially influences the composition.
- Iron segregated the most.
- Cobalt desegregated the most.
- Composition comes to a steady state

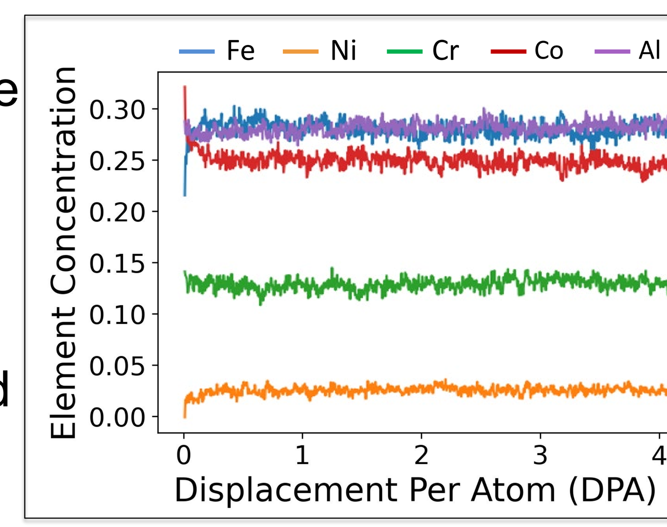
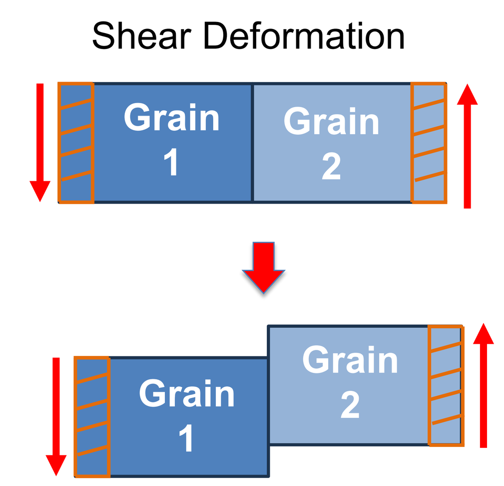


Figure 6. Change of concentration with irradiation

Shear testing Irradiated and Non-irradiated Structures

- Study effect of irradiation on mechanical properties
- Method: Applied athermal shear deformation
- Strain magnitude per minimization step: 0.04 Å



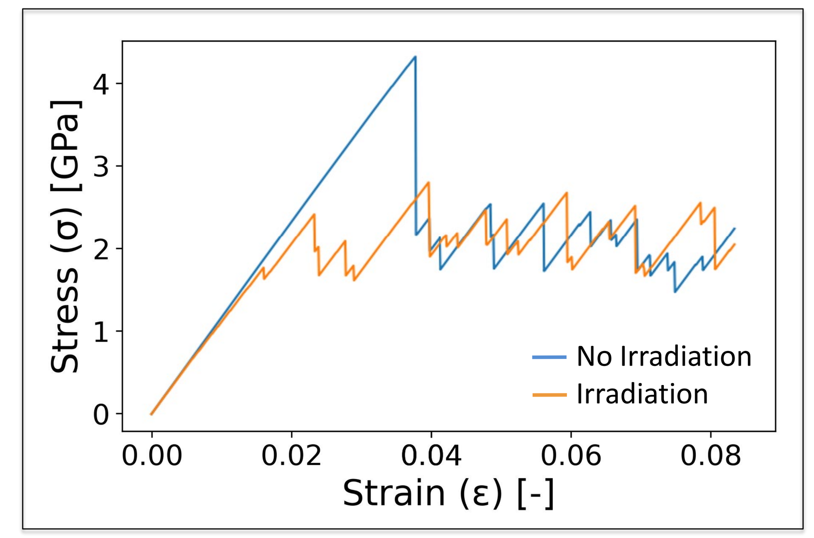


Figure 7. Stress Strain Response

- Irradiated structure has a smaller yield strain and yield stress
- Radiation makes the GB weaker under shear
- Flow stress at steady state is similar

Conclusion

- Atomistic simulations were used to analyze if irradiation leads to quantifiable steady state disordered GB structures.
- GB core comes to a steady state and becomes radiation resistant.
- Radiation leads to a weakened GB and weakened mechanical properties

References

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Acknowledgements

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