High-dose damage evolution in Fe, FeCr and high-entropy alloys

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Arcing experiments
1. Damage overlap effects
   - Experimental basic knowledge
   - Early MD simulations
   - Simulation of massive damage overlap: Si, metals
2. High-dose damage in high-entropy alloys
   - Explanation to high radiation hardness
3. High-dose damage effects in Fe and FeCr
   - Mechanism of 100 loop formation
Molecular dynamics of primary damage event

- The primary damage (ns timescale) produced by neutron irradiation can be readily simulated by molecular dynamics (=simulation of atom motion)

- Simple example: 10 keV recoil cascade in FeCr, cross-sectional view
1. Overlapping damage effects?

- It is well established that overall damage levels in metals saturate on long-term irradiation
- Basic explanation: new cascades recombine some of old damage
- Saturation at ~ 1% defect concentration


**Experiment**

![Graph showing damage effects in copper](image1.png)

[Copper](image2.png)


**Simulation**

![Simulation of damage effects](image3.png)

Simulations of high-dose damage in semiconductors

- High-dose damage can be simulated by molecular dynamics by running repetitive cascades in same cell
- If there is no thermally assisted defect migration, this corresponds directly to high-dose radiation experiments
- For semiconductors such simulations have been done already long ago, and gave good agreement with experiments
- E.g. amorphization of silicon
  - Dose about 14 eV/atom in MD, about 12 eV/atom in expt.

Simulations of high-dose damage in metals

- Until recently, there were no corresponding simulations in metals
- We have now carried out numerous such series in Fe, FeCr, Ni and Ni-related high entropy alloys
- Example: 1500 overlapping 5 keV cascades in Ni
- 108000 atom cell, all atoms plotted in projection

Granberg et al. (2015)
2. High-Entropy and Equiatomic multicomponent Alloys

- High-entropy (HEA) and Equiatomic MultiComponent (EAMC) alloys are metal mixtures with multiple elements at equal or roughly equal concentrations, homogeneously distributed, in a single simple crystal.

- Definitions:
  - HEA: 5 or more elements
  - EAMC: 2 or more elements

- Rapidly rising interest to them due to promising mechanical, corrosion-resistant and radiation hardness properties
Damage in high-entropy alloys?

- Experiments by Yanwen Zhang et al (ORNL) show that damage in some FCC high-entropy alloys can be clearly lower than in the corresponding pure elements.
- Standard point of comparison: Ni, which is already quite radiation-hard.

![Graph showing yield vs. depth for different materials at 1.5 MeV Ni.]

- Amorphous level
- Damage free level
- Yield (a.u.)
- Depth (nm)

Single cascades in HEA’s

- It is not *a priori* clear why damage should be lower in high-entropy alloys
- Some alloys, such as NiAl, amorphize on irradiation!
- Single cascades in HEA’s do not really show a difference to pure elements
- Example: 5 keV cascade in model CoNiFeCr HEA:
  - Recombination as usual, very similar to pure Ni
  - Damage slightly *higher* than in Ni
- Cannot explain experiments – something else is needed
To try to understand the damage saturation effects in HEA’s, we ran > 1500 overlapping cascades in them.

Key observation: after about 0.05 dpa, almost all damage is in clusters – and this evolves!

Example: FeNi

The clustered damage shows a similar damage reduction effect as the experiments!

Experiment (RBS)

Simulation (MD)

Analyses of dislocation structures

- We have analyzed all the frames for dislocations with the ovito DXA analysis (constructing Burgers vectors to detect dislocations)

- Ni

- NiCoCr

Stair-rod dislocation => Stacking fault tetrahedron

Shockley partial

Frank loop
Final dislocation state
Ni vs. NiCoCr

- Ni has larger dislocation loops and much more SFT’s than NiCoCr

Ni ~ 0.3 dpa
NiCoCr ~ 0.3 dpa
Dislocation reactions affecting overall damage level

- The dislocations dominate the overall damage level
- Numerous dislocation reactions occur driven by the irradiation
- Example: Shockley partial stepwise becoming a Frank loop
Reason to damage reduction: reduced dislocation mobility

- The reduction in damage level correlates clearly with dislocation mobility
- In the alloys, each atom has a local strain field, and this reduce dislocation mobility
- Lower dislocation mobility keeps dislocations from growing, and the smaller dislocations can recombine easier during cascade overlap

Final damage level vs. Slope of dislocation mobility => Clear correlation

Why is RBS signal so high?

- In the experiments, the RBS/channeling signal appears very high, about "1/2 randomly displaced atoms"
- 50% damage does not at all correspond to TEM, resistivity or MD results, which show <1% defective atom fraction
- Explanation just determined by us: dislocations give a very high RBS signal due to strain effects
- New code RBSADEC to simulate RBS/channeling from arbitrary atom coordinates shows that signal from loop ~50x higher than for same number of randomly displaced interstitial atoms!

Direct comparison of damage structure with experiments

- Using the RBSADEC code we can compare our structures directly with experiments (with no fitting!)
- Agreement is very good considering defect migration is not included in MD simulations and we use a single ion energy

3. High-dose radiation damage in Fe and FeCr

- We have also carried out corresponding series in Fe
- Key question addressed in these simulations: what is the mechanism of 100 loop formation?
Dislocation structure after 1000 5 keV cascades

½ <111> dislocation
<100> dislocation
Unidentified; mainly vacancy clusters
100 loop formation mechanism

- From the simulations, we analyzed the dislocation structure [with Ovito DXA analysis] and sought 100 loops
- We found that they can form spontaneously by transformation from 111 loops by cascade overlap
- Example:

  ![Diagram](image)

  - (a) Before cascade 1026
  - (b) After cascade 1026
  - (c) Before cascade 1288
  - (d) During cooldown
  - (e) During cooldown
  - (f) After cascade 1288

[Granberg et al, EPL (2017) submitted for publication]
Video of final transformation

Note time scale: final loop transformation occurs after heat spike: spike ‘activates’ a locked-in dislocation configuration
Another case…

- Transformation of final $<111>$ segment to $<100>$

- Note time scale: final loop transformation occurs after heat spike: spike ‘activates’ a locked-in dislocation configuration
Conclusions

- Dislocation mobility is reduced in FCC high-entropy alloys
- After about ~ 0.05 dpa, overall damage level is dominated by dislocation structures, and their reactions affect the development
- This reduces the radiation damage in high-entropy alloys compared to the corresponding pure elements
- In Fe, <100> loops can form stepwise by cascade-induced activation of <111> dislocation segments
Thank you for your attention!