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

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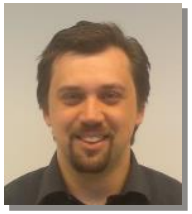

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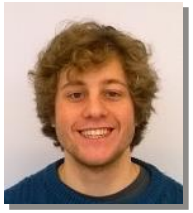

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Arcing experiments

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3. High-dose damage effects in Fe and FeCr
   - Mechanism of 100 loop formation

Molecular dynamics of primary damage event

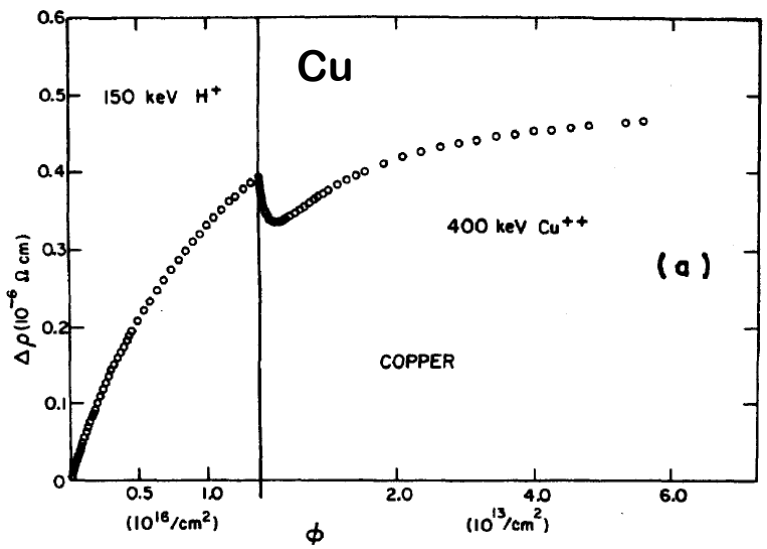
- The primary damage (ns timescale) produced by neutron irradiation can be readily simulated by molecular dynamics (=simulation of atom motion)
- Simple example: 10 keV recoil cascade in FeCr, cross-sectional view

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

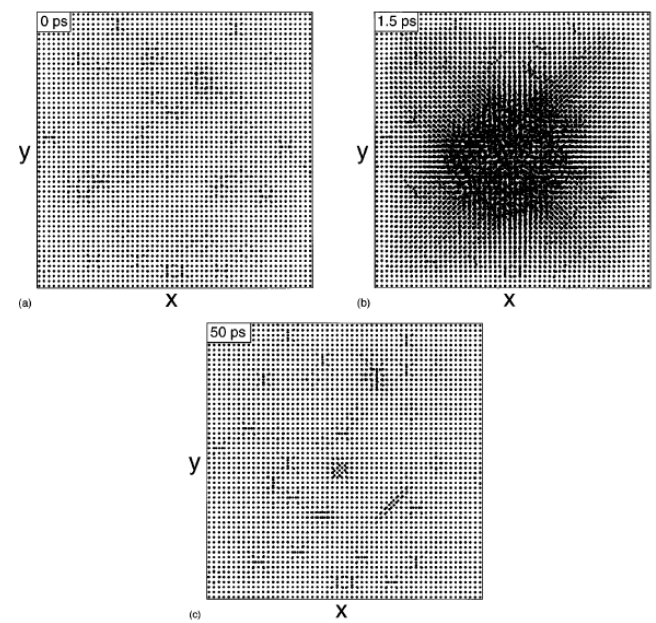
    [Gao, Bacon et al, J. Nucl. Mater. 230 (1996) 47; Nordlund and Averback, Phys. Rev. B 56, 2421 (1997)]

Experiment



[Averback et al,. Phys. Rev. B 16 (1977) 3860]

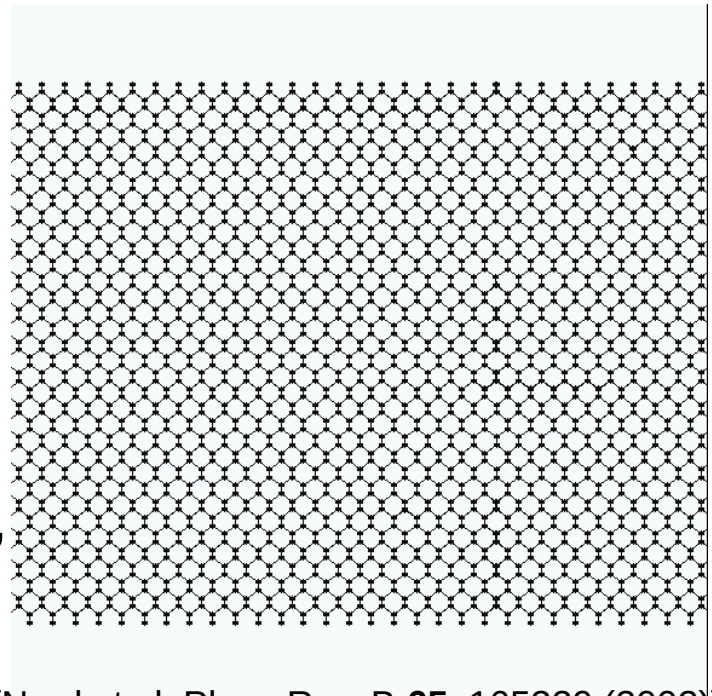
Simulation



[Nordlund and Averback, Phys. Rev. B 56, 2421 (1997)]

Simulations of high-dose damage in semiconductors

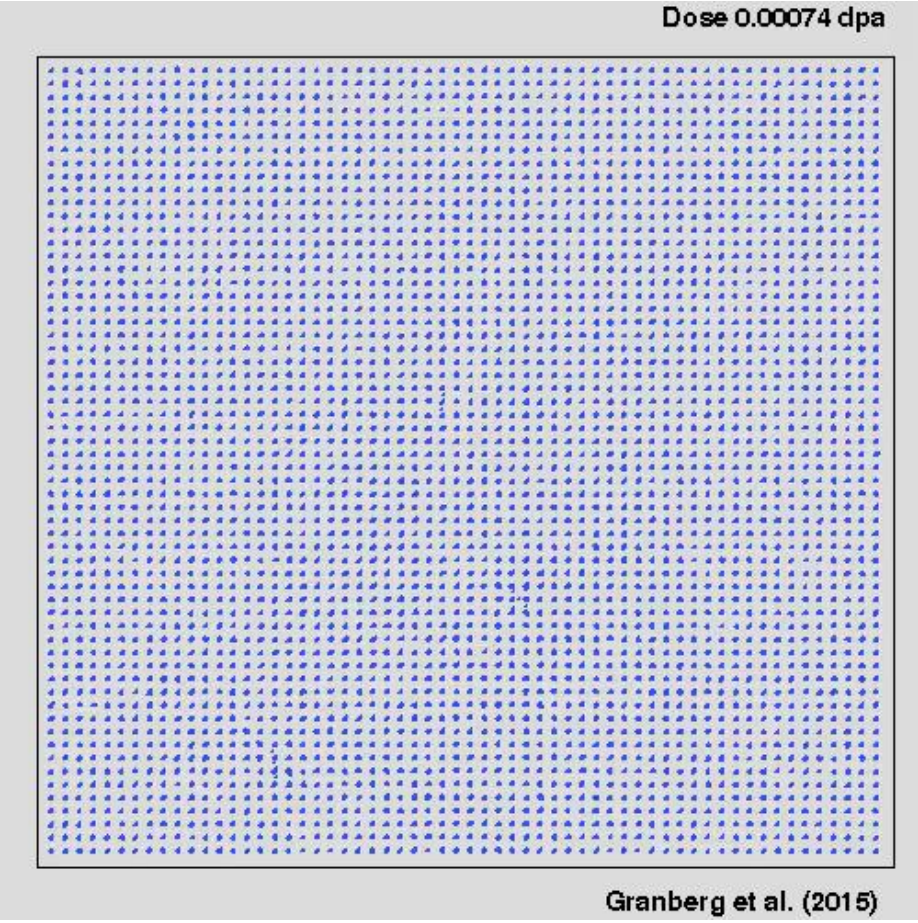
- High-dose damage can be simulated by molecular dynamics by running repetitive cascades in same cell
  - If there is no thermally assisted defect migration, this corresponds directly to high-dose radiation experiments
- For semiconductors such simulations have been done already long ago, and gave good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



[Nord et al, Phys. Rev. B **65**, 165329 (2002)]

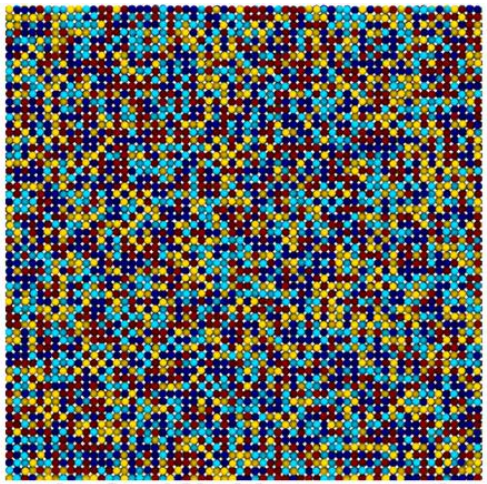
Simulations of high-dose damage in metals

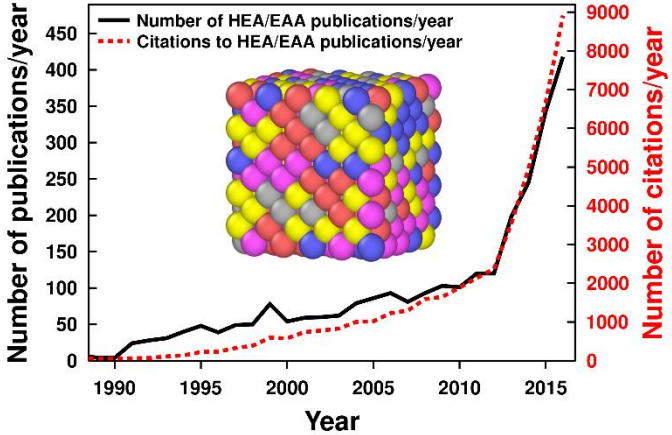
- Until recently, there were no corresponding simulations in metals
- We have now carried out numerous such series in Fe, FeCr, Ni and Ni-related high entropy alloys
- Example: 1500 overlapping 5 keV cascades in Ni
  - 108000 atom cell, all atoms plotted in projection



2. High-Entropy and Equiatomic multicomponent Alloys

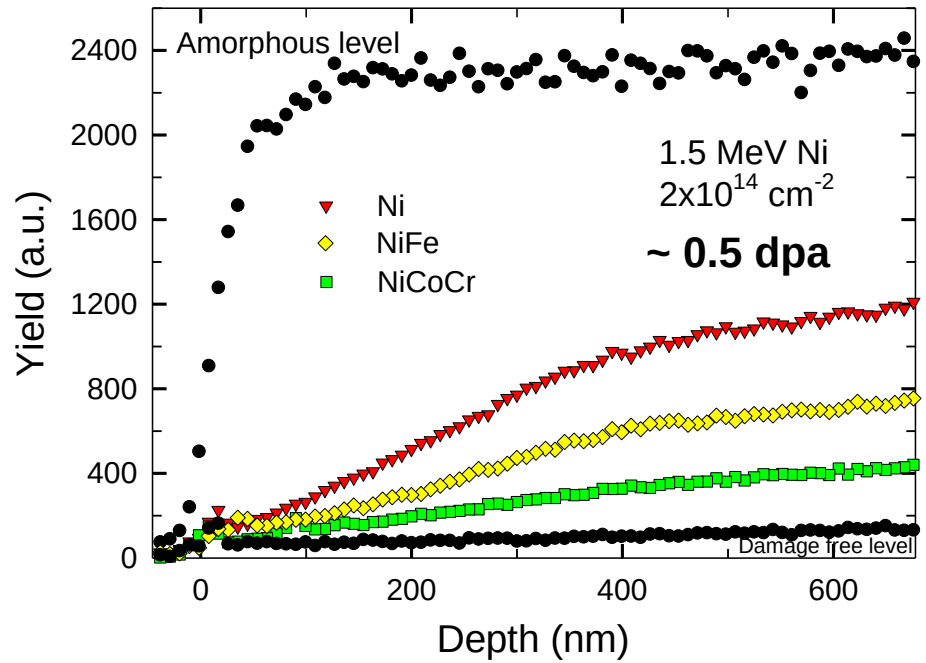
- High-entropy (HEA) and Equiatomic MultiComponent (EAMC) alloys are metal mixtures with multiple elements at equal or roughly equal concentrations, homogeneously distributed, in a single simple crystal
  - Definitions:
    - HEA: 5 or more elements
    - EAMC: 2 or more elements
- Rapidly rising interest to them due to promising mechanical, corrosion-resistant and radiation hardness properties





Damage in high-entropy alloys?

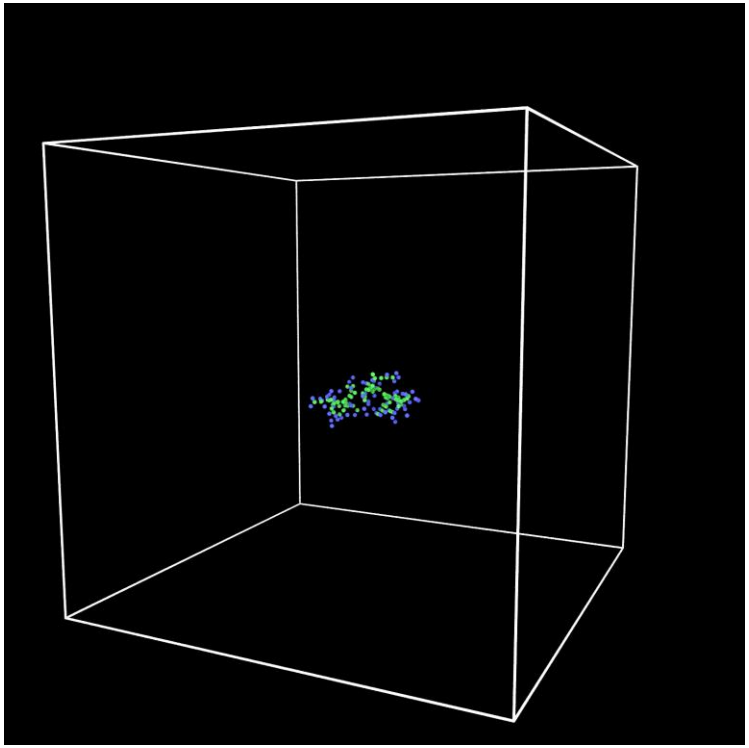
- Experiments by Yanwen Zhang *et al* (ORNL) show that damage in some FCC high-entropy alloys can be clearly lower than in the corresponding pure elements
  - Standard point of comparison: Ni, which is already quite radiation-hard



[Granberg, Nordlund, Zhang, Djurabekova et al, Phys. Rev. Lett. 116, 135504 (2016).

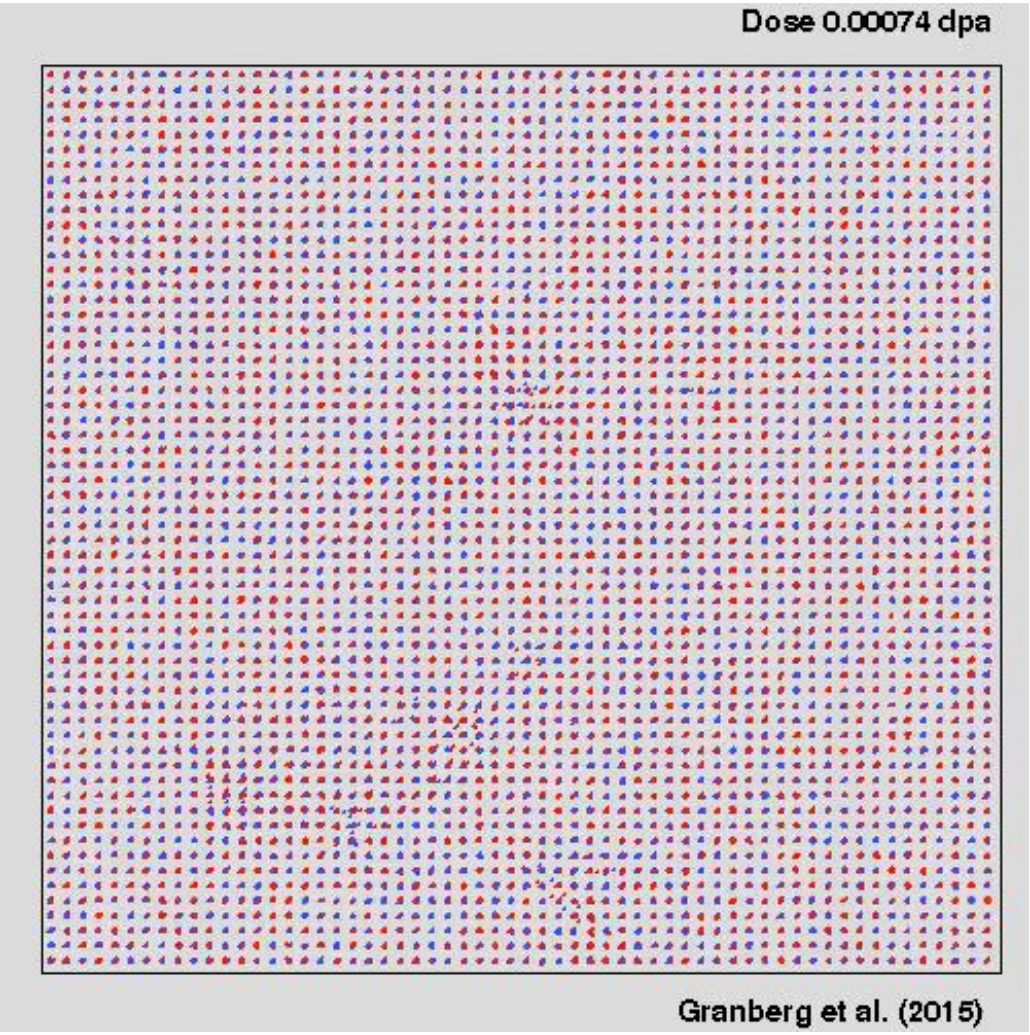
Single cascades in HEA's

- 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



Damage overlap effects in HEA's

- 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

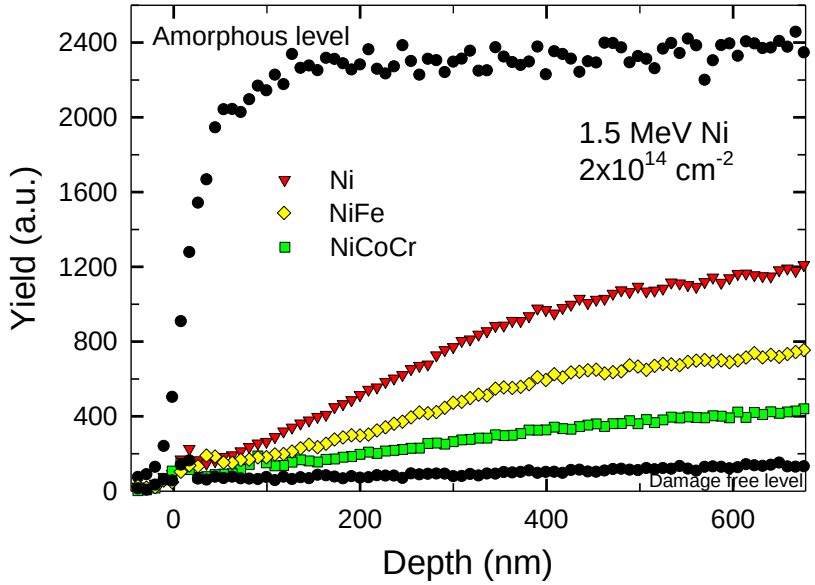


[Granberg, Nordlund, Zhang, Djurabekova et al, Phys. Rev. Lett. 116, 135504 (2016).

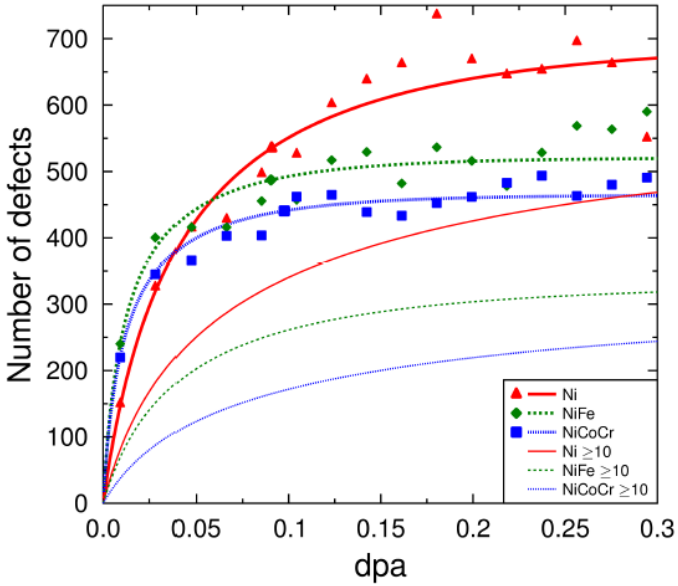
Damage in clusters in HEA's

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

Experiment (RBS)



Simulation (MD)



[Granberg, Nordlund, Zhang, Djurabekova et al, Phys. Rev. Lett. 116, 135504 (2016)]

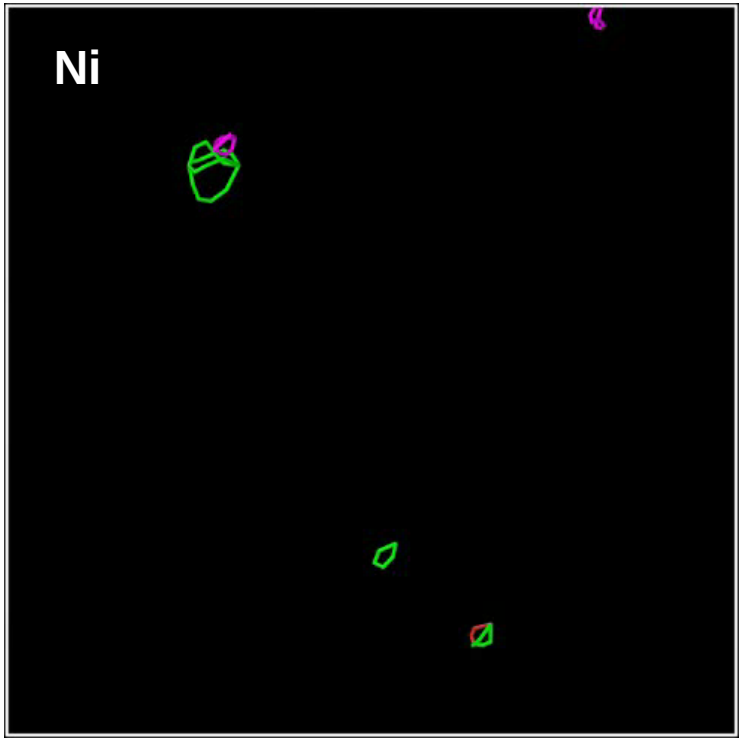
Analyses of dislocation structures

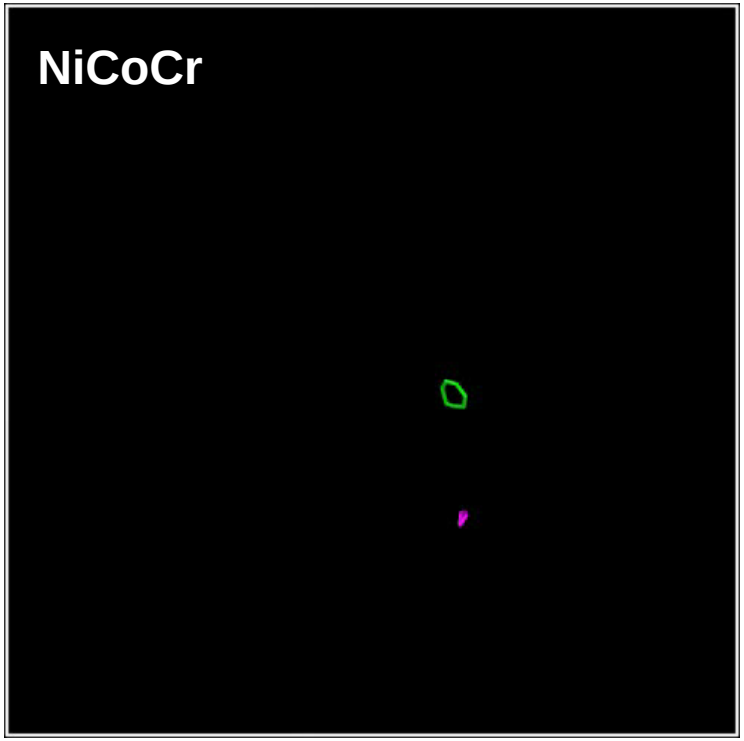
- We have analyzed all the frames for dislocations with the ovito DXA analysis (constructing Burgers vectors to detect dislocations)

Stair-rod dislocation => Stacking fault tetrahedron

Shockley partial

Frank loop

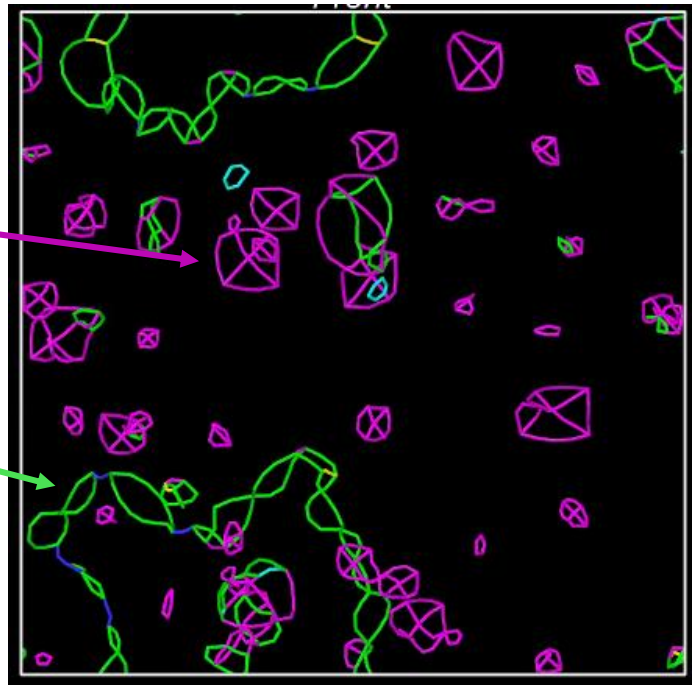




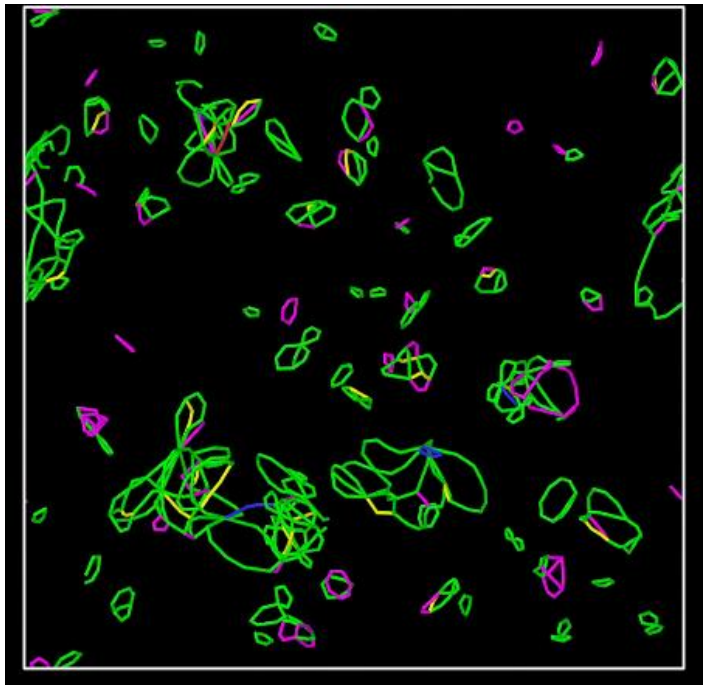
Final dislocation state Ni vs. NiCoCr

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

Ni ~ 0.3 dpa



NiCoCr ~ 0.3 dpa



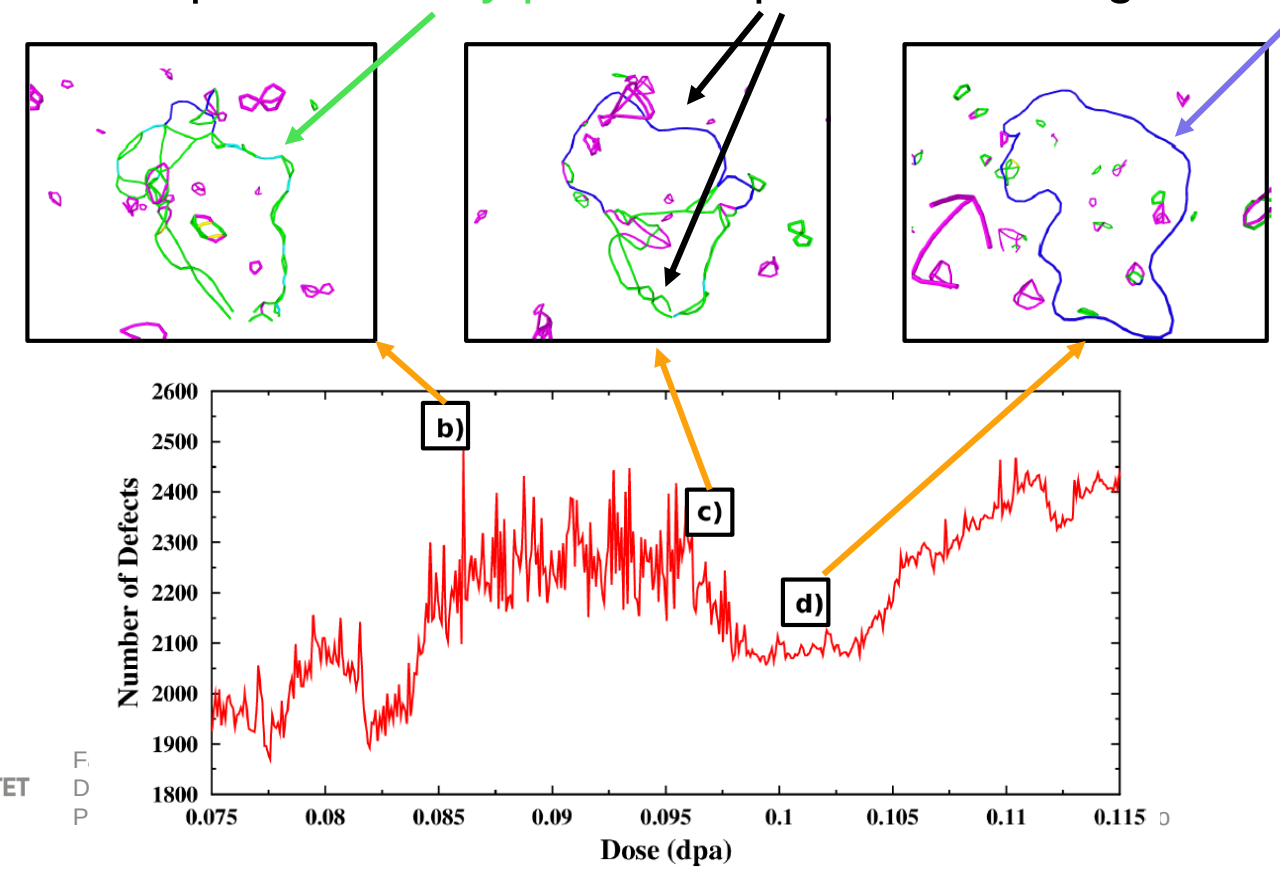
Stacking fault tetrahedron

Shockley partial

Frank loop

Dislocation reactions affecting overall damage level

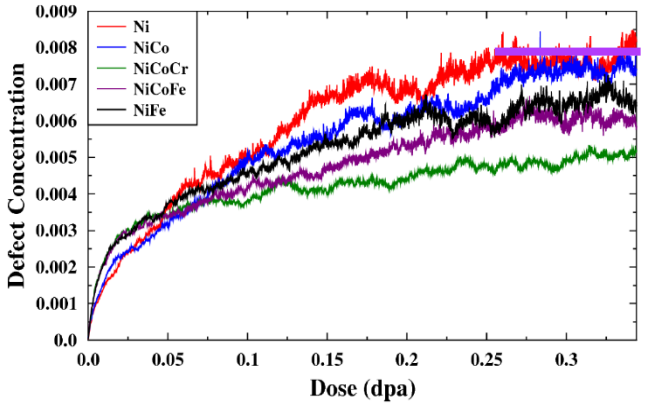
- The dislocations dominate the overall damage level
- Numerous dislocation reactions occur driven by the irradiation
- Example: Shockley partial stepwise becoming a Frank loop

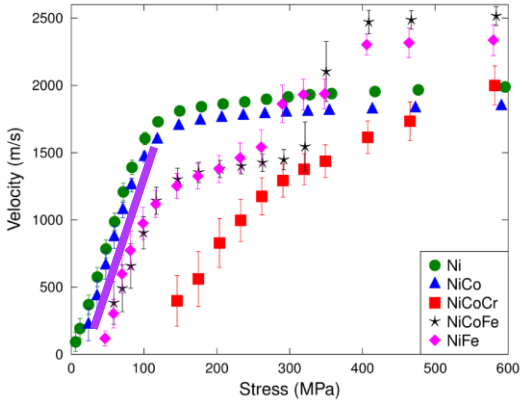


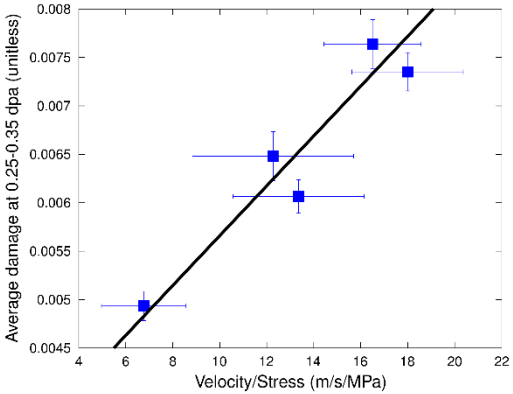
Reason to damage reduction: reduced dislocation mobility

- 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



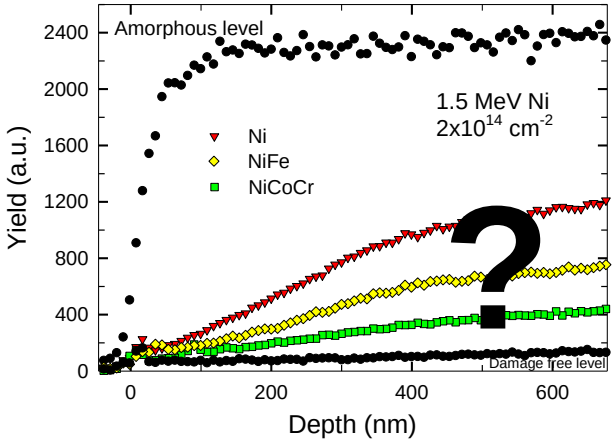


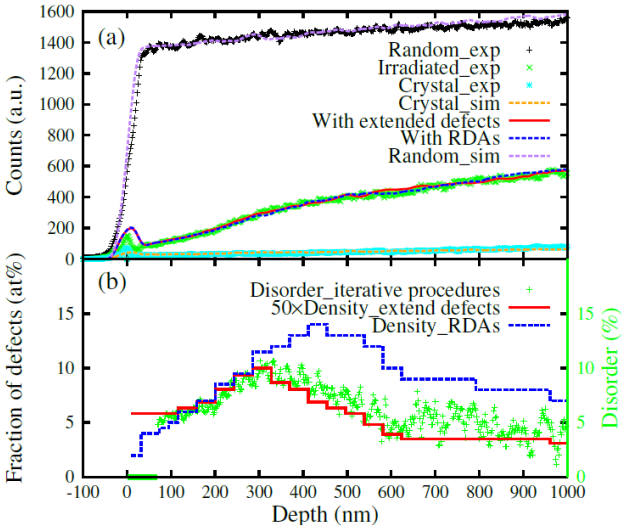


[Granberg et al, Nucl. Instr. Meth. B (2017), accepted]

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!





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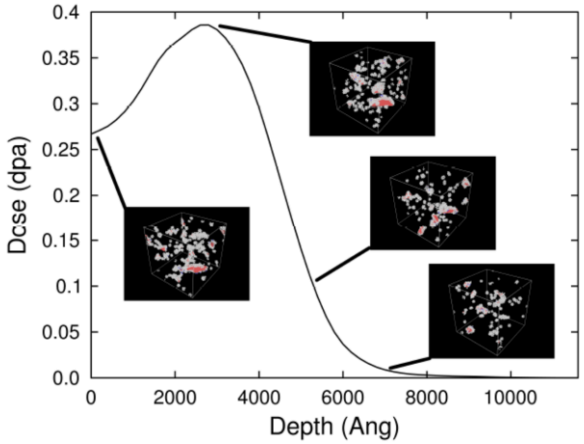
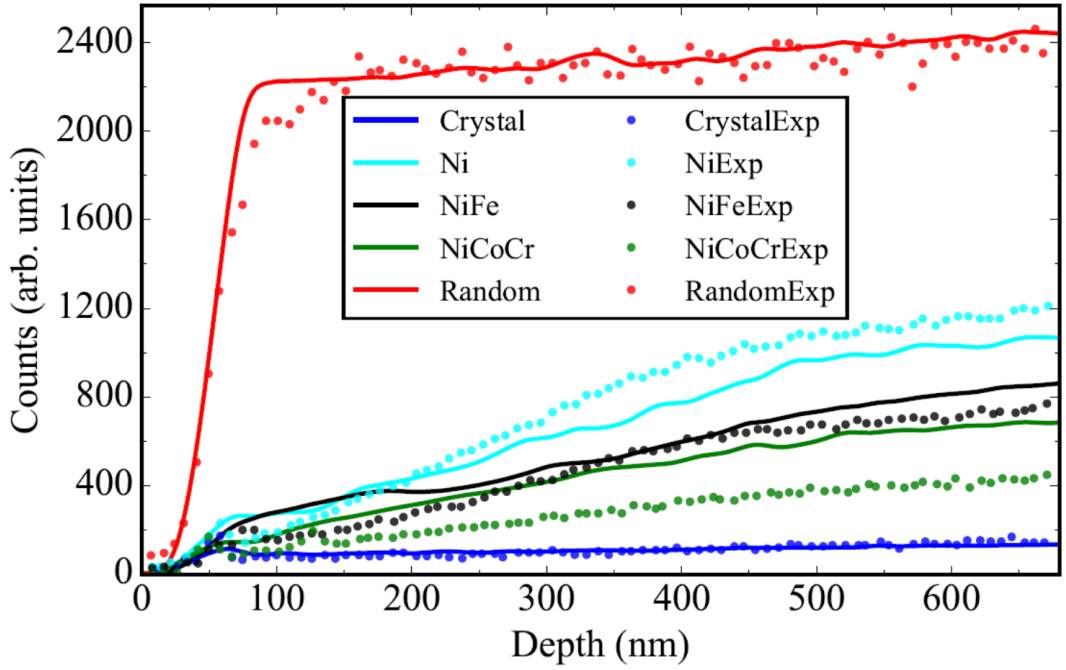
Prof. Kai Nordlund

[S. Zhang, K. Nordlund, F. Djurabekova, Y. Zhang, G. Velisa, and T. S. Wang, Phys. Rev. E 94 (2016) 043319]

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

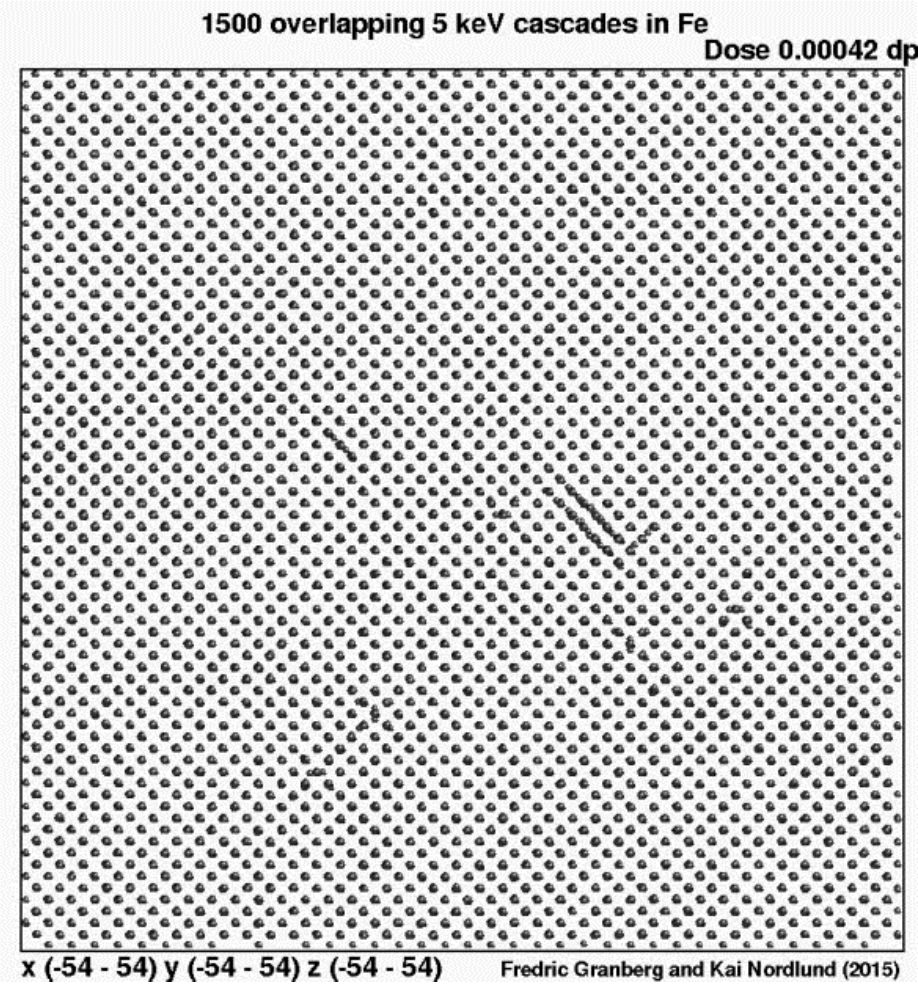




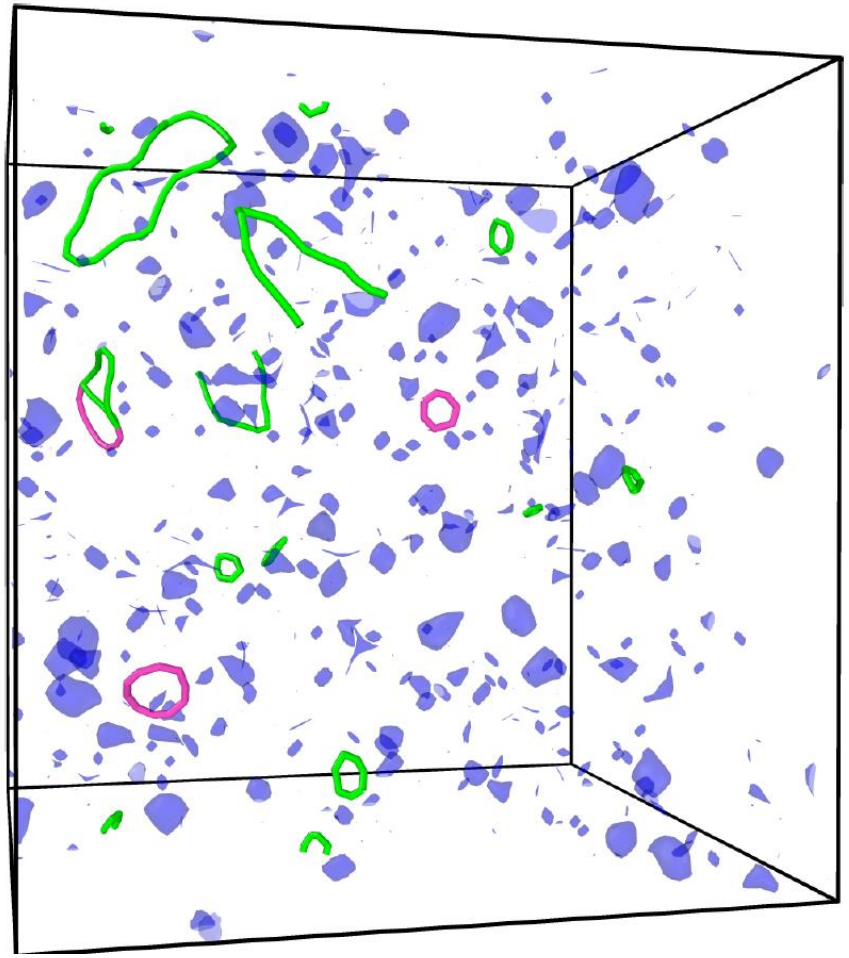
[S. Zhang, K. Nordlund, F. Djurabekova, F. Granberg, Y. Zhang, and T. S. Wang, Mater. Res. Lett. (2017) accepted]

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?



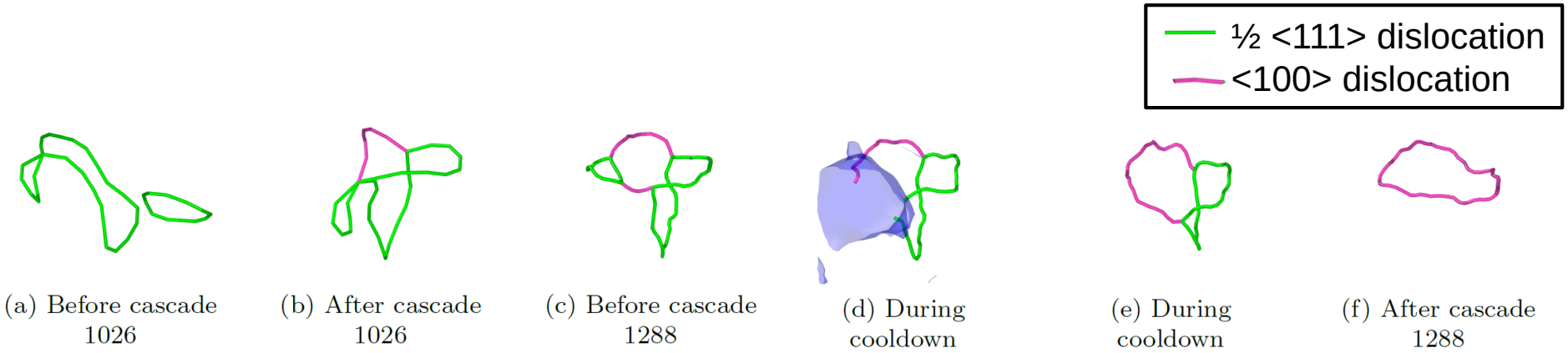
Dislocation structure after 1000 5 keV cascades



½ <111> dislocation
<100> dislocation
Unidentified; mainly vacancy clusters

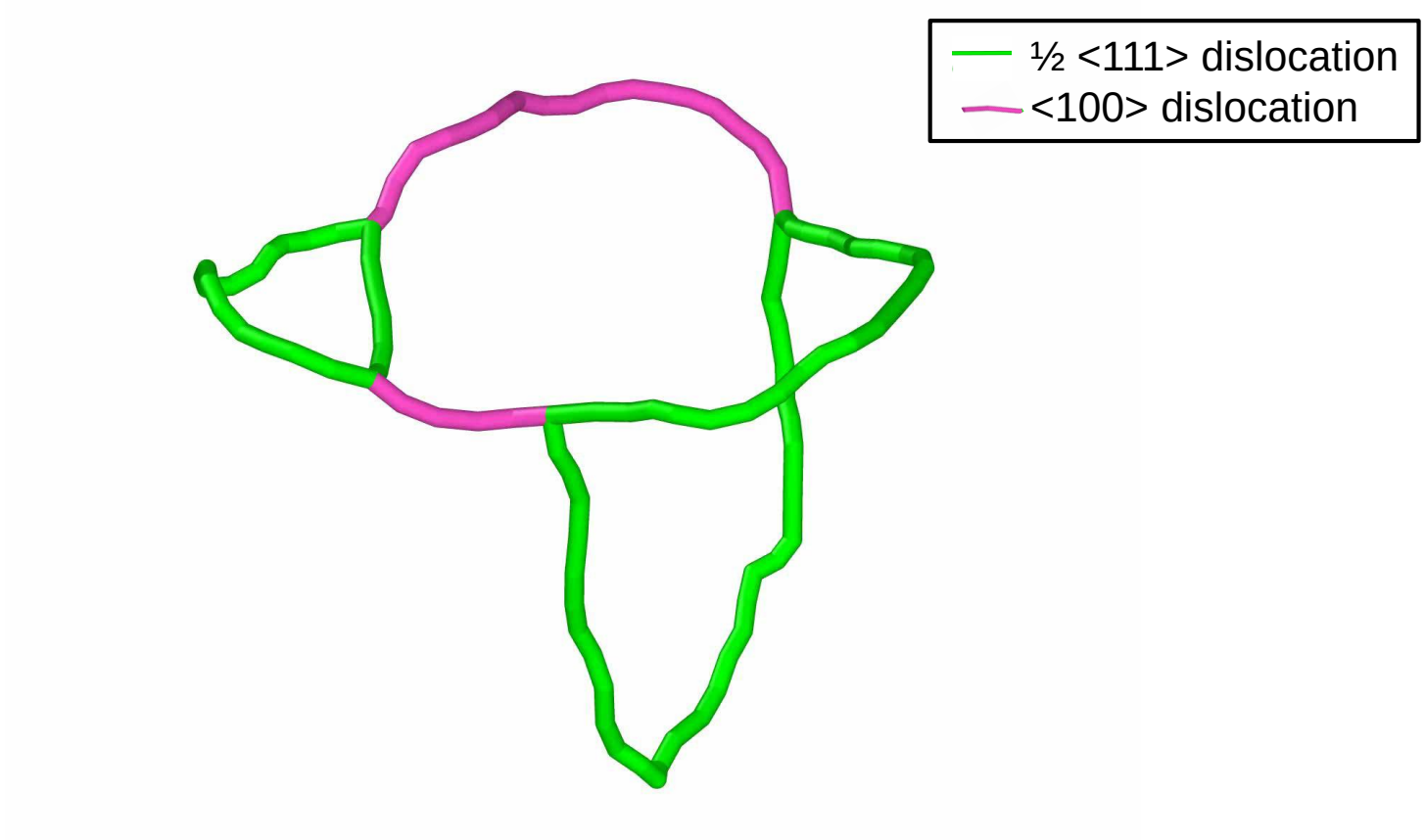
100 loop formation mechanism

- 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:



[Granberg et al, EPL (2017) submitted for publication]

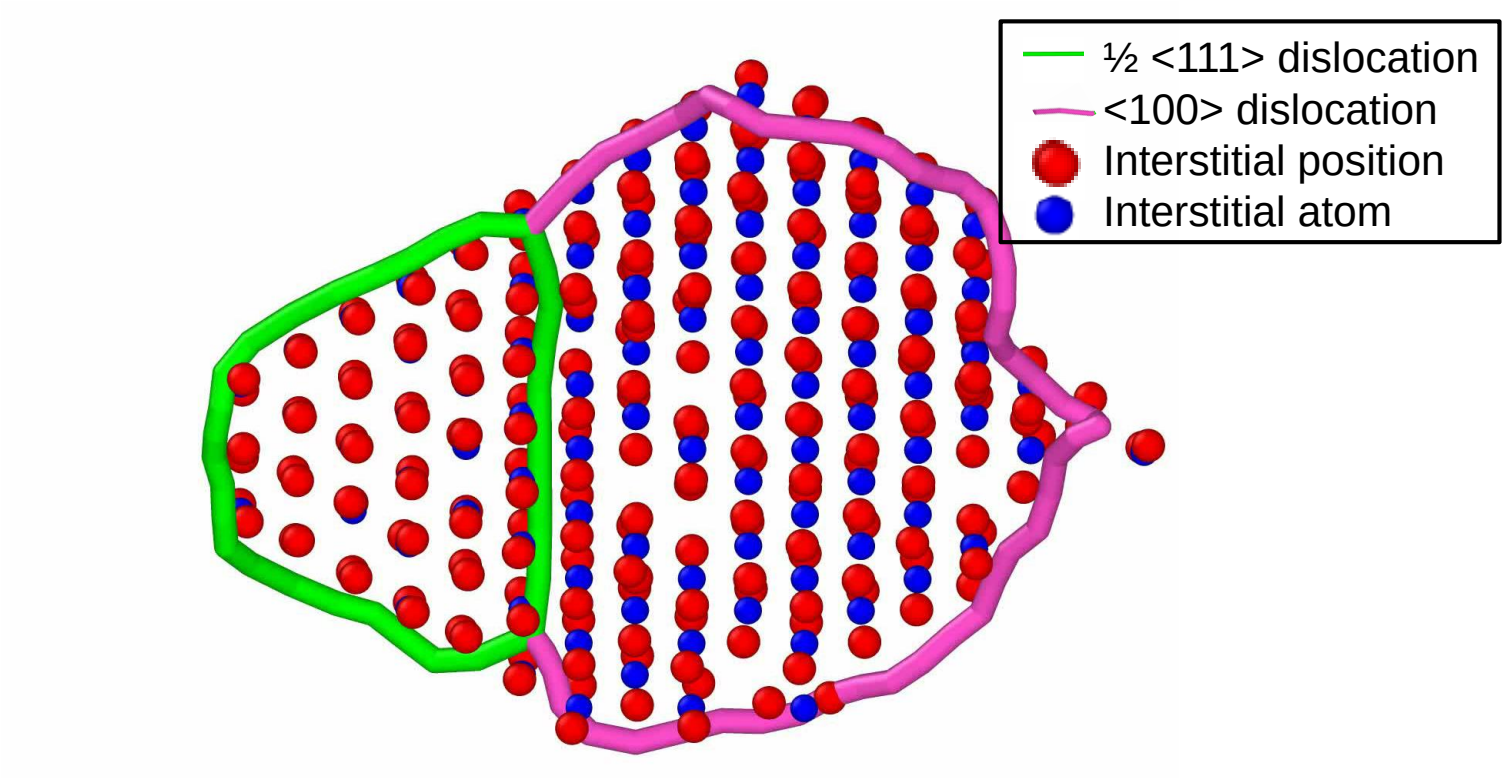
Video of final transformation



- 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 you attention!