Crack healing induced by collision cascades in Nickel

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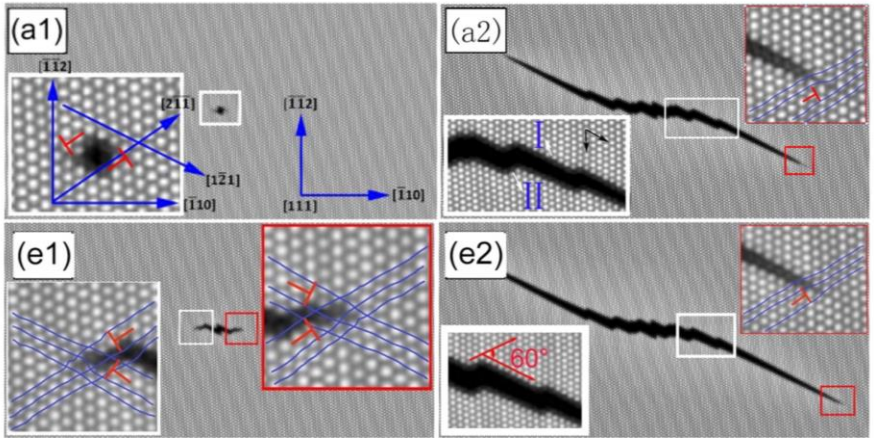
Motivation

- Nanoscale cracks could be inadvertently introduced into materials during processing or in service.

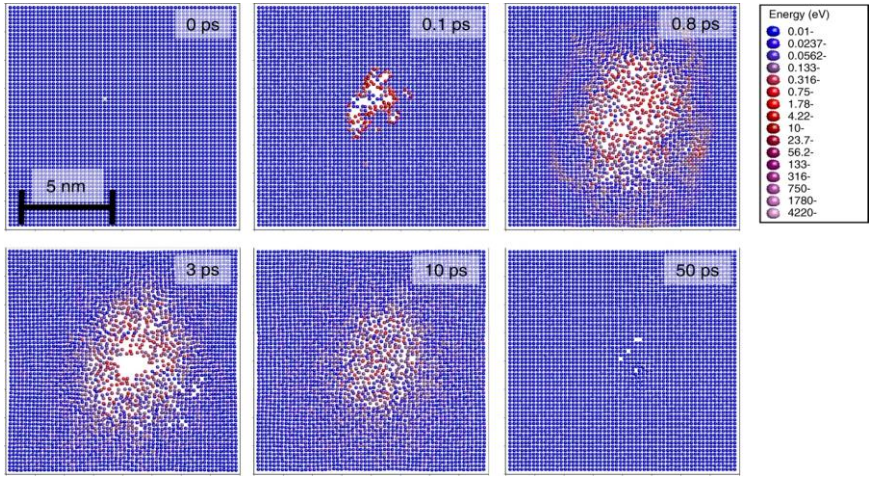
The crack propagation in nanoscale under strain



Gao et al. / Computational Materials Science, 2017

- Metallic structural components in nuclear reactors are exposed to radiation damage.

Atomistic simulation of radiation-induced defect creation



Nordlund et al. / Nature Communications, 2018

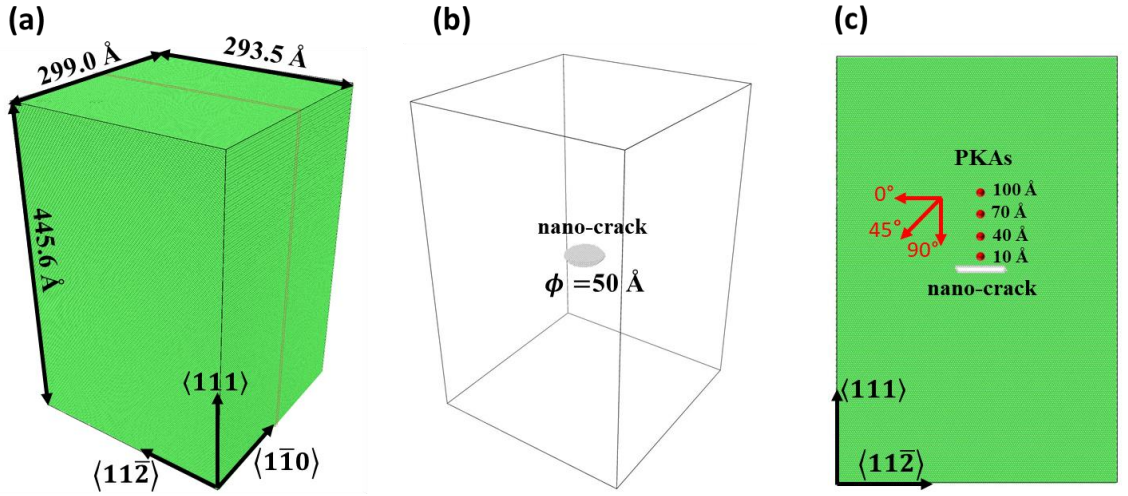
For the structural metallic material in nuclear power engineering, such as nickel, the interaction between nanoscale crack and collision cascade is inevitable.

Questions:

1. **How collision cascades and the generated damage affect structure of nanoscale cracks?**
2. **How crack influences the collision cascade and the formation of radiation damage?**

Simulation methodology

- **HPRC cluster: Ada**
- **LAMMPS for MD simulation**
- **Ovito for visualization**



Configuration of simulation cell—Ni single crystal with a nanoscale crack

Simulation setup:

1) A nanoscale crack (ϕ =50 Å) is introduced at the center of simulation cell, crack surface ∥ {111} plane.
2) The collision cascade is initiated by imparting a kinetic energy to a primary knock-on atom (PKA). Four scenarios: different distances of PKA above the crack—10, 40, 70 and 100 Å; for each scenario three different PKA directions —0°, 45° and 90° are further considered.

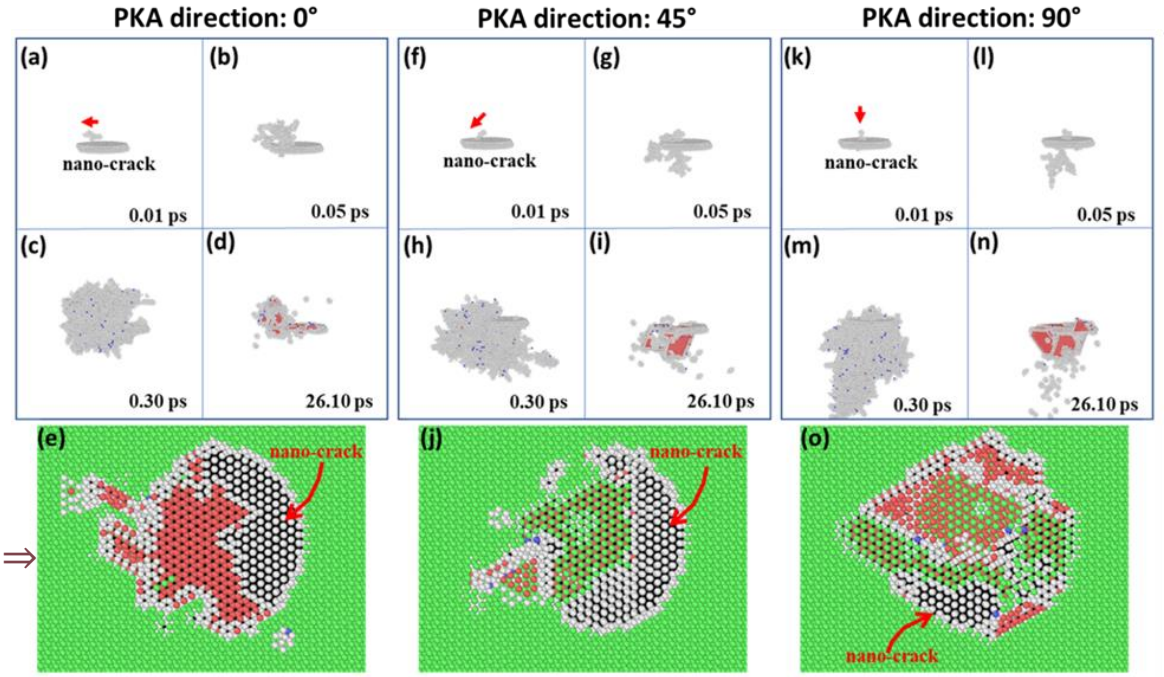
As such, the interaction between collision cascade and crack can be investigated, the effect of PKA positions and velocity directions can also be studied.

Results: collision cascade induced-crack healing

Collision cascade:

1. **0.01 ps:** ballistic phase
2. **0.05 ps:** collision cascade spreads out
3. **0.30 ps:** thermal spike core expands to its maximum size
4. **26.10 ps:** collision cascade has already cooled down to equilibration

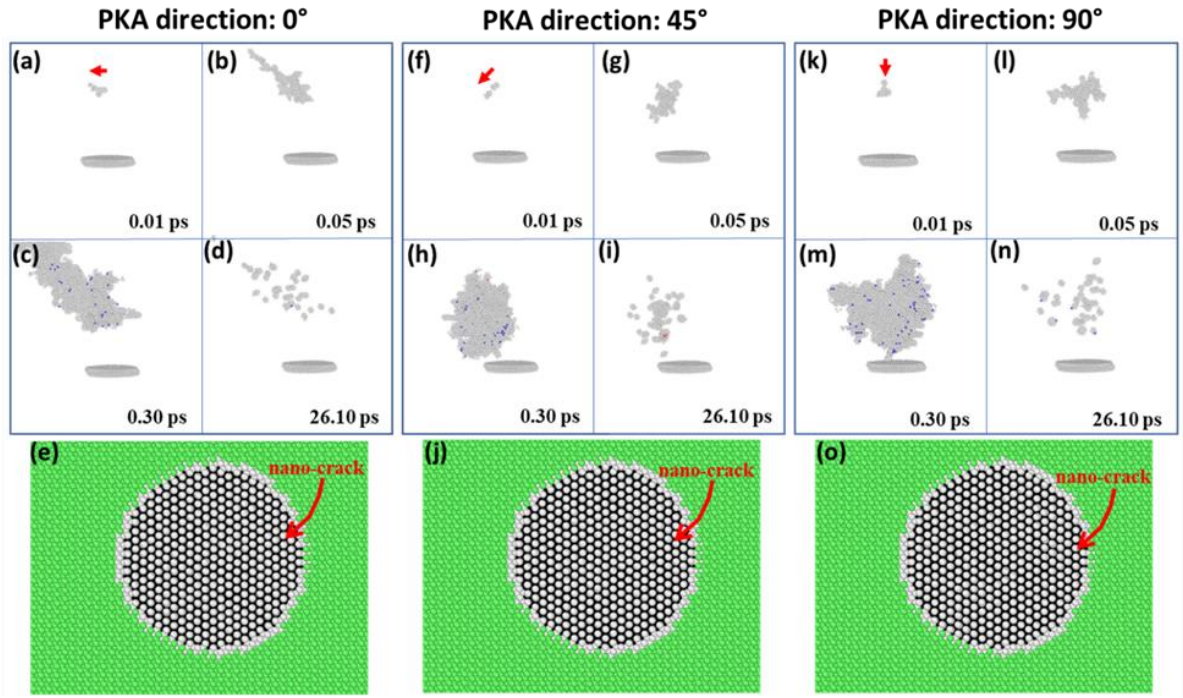
➢ **PKA distance=10 Å; kinetic energy=10 keV**



Representative snapshots of the microstructural evolution at different times

- ❑ **the thermal spike core grows to maximum size and overlaps with crack, and the crack can be partially healed**
- ❑ **dislocation loops and stacking faults are generated after equilibration**

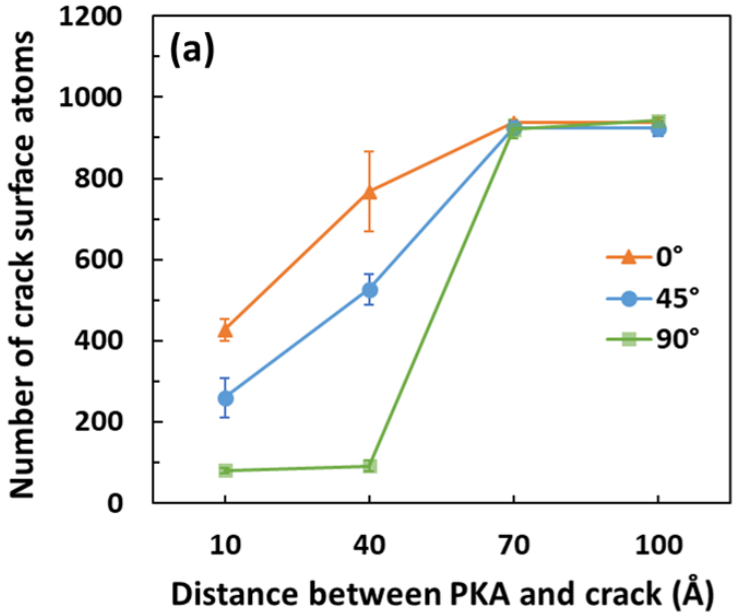
➢ **PKA distance=70 Å; kinetic energy=10 keV**



Representative snapshots of the microstructural evolution at different times

- ❑ **Irrespective of PKA directions, no overlapping between crack and thermal spike core occurs, and no crack healing is observed**
- ❑ **After equilibration, the radiation damage is mainly in the form of point defects, almost no dislocation loop and stacking fault can be observed**

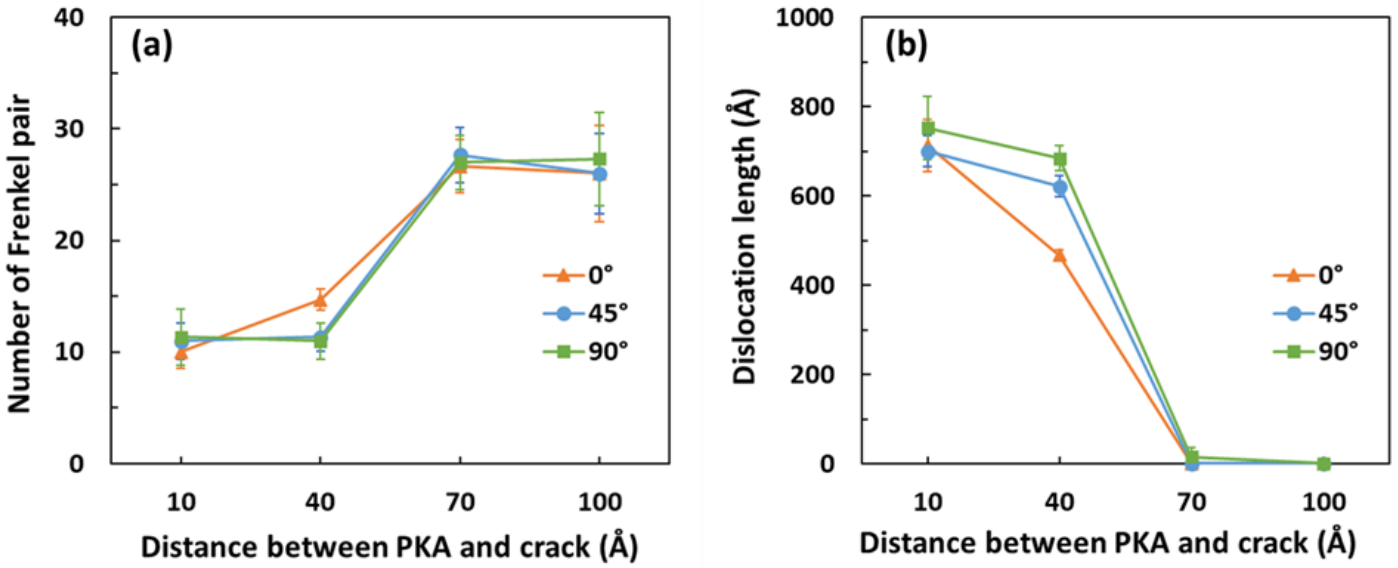
Trends in cascade-induced crack healing



Reduction of crack surface area varies markedly with both PKA direction and distance:

- as the PKA distance is increased, the number of crack surface atoms also increases, indicating the crack is more difficult to be closed.
- the 90° direction is more effective in healing the crack than the 0° and 45° directions, due to the larger fraction of overlapping crack area with thermal spike core.
- Once the PKA distance is greater than 70 Å, no crack healing can occur, due to the thermal spike does not overlap with the crack..

Trends in cascade-induced crack healing



- the number of Frenkel pairs is significantly increased when the PKA distance is increased from 40 Å to 70 Å.
- When crack overlaps with thermal spike core (at 10 Å and 40 Å), a considerable amount of dislocations are activated. However, the dislocation length is nearly zero when no overlapping occurs

Discussion and Summary

- ✓ **Collision cascade induced-crack healing:** the crack can be healed when crack overlaps with a thermal spike core and remains intact when no overlapping occurs.

- ✓ **The overlapping of crack with thermal spike core affects the radiation induced-defects:** dislocation loops and stacking fault tetrahedra dominate when the crack overlaps with thermal spike. However, the point defects dominate when no overlapping occurs.