Modelling the Effect of Helium bubbles, Rigid Inclusions and Grain Boundaries on Crack Initiation in Nickel

Tung Yan Liu, Michael J. Demkowicz
Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843, USA

**Motivation**
- Inter-granular fracture is observed in irradiated nickel(Ni)-based Inconel X-750 spacers.
- How do cracks form in initially flaw-free Inconel X-750?

**Hypothesis:** cracks initiate at slip bands interacting with He bubbles

Our goal: test this hypothesis via large-scale atomistic simulations of Ni with irradiation defects

**Modelling irradiation defects**
- 0.04% Ni self-interstitial atoms (SIAs) are added to FCC Ni and allowed to cluster under 1000K annealing.
- Models with a target density of bubbles are generated according to experimental data.

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<th>SIA clusters*</th>
<th>He-filled bubbles* with GB &amp; inclusion*</th>
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Illustrations from: *small model: ~100K Ni atoms, ~10nm x 10nm x 10nm
*large model: ~10M Ni atoms, ~48 nm x 50 nm x 50 nm

**Mechanical Loading**
- The choice of loading state reduces chances of hardening and thereby promotes slip band formation.
- Apply 1000 strain increments with strain ~ 0.0001 (0.01%) total strain = ~0.1 (10%) Relax using MD at T = 588K for 0.1ns per increment total length of each simulation = 100ns - strain rate = 10\(^6\)/s

**SC model gives larger stress drops than the GB models**

**Conclusions: what about cracks?**
- No crack is observed at slip bands forming in our model.
- Next step: slip vector and bubble analysis on all large models.

**High performance computing summary**
- Implemented using LAMMPS on ADA and TERRA at HPRC.

- Small 100K atoms: 320 cores, 2.5G memory ~48 hrs (ADA).
- Large 10M atoms: 512 cores (GPU nodes), 8G memory for ~1224 hrs (TERRA).

**Shearing of He bubbles**
Dislocations cut through bubbles during stress drops

**Dislocation impart permanent shape change to He bubbles**

**Snapshots from small model:~100K Ni atoms, ~10nm x 10nm x 10nm**

**Slip Band Formation**
A slip band with dislocations gliding on the (1,1,1) plane is observed in SC model; bubbles along the band are severely strained.