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

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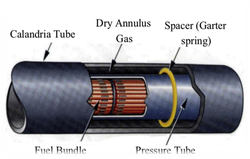
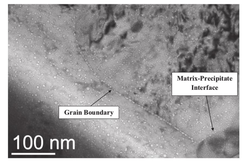
Motivation

- 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?





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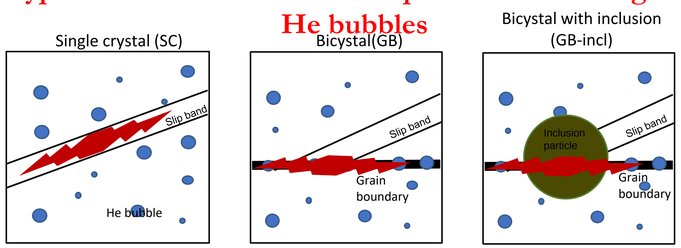
Hypothesis: cracks initiate at slip bands interacting with He bubbles

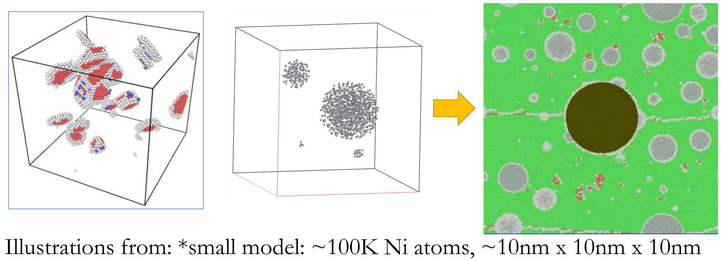


Our goal: test this hypothesis *via* large-scale atomistic simulations of Ni with irradiation defects

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

SIA clusters* | He-filled bubbles* | with GB & inclusion^



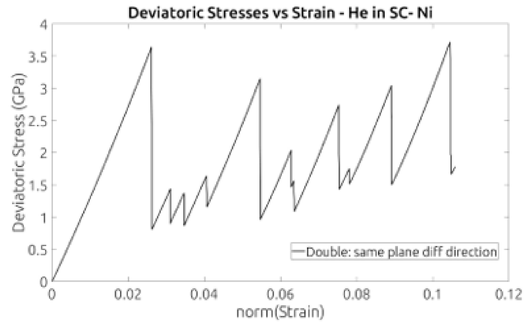
Illustrations from: *small model: ~100K Ni atoms, ~10nm x 10nm x 10nm
^large model: ~10M Ni atoms, ~48 nm x 50 nm x 50 nm

Acknowledgements

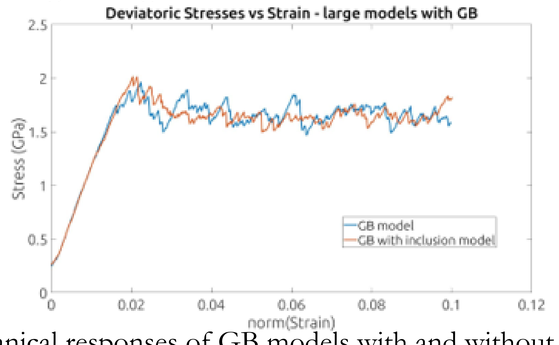
- This project is funded by the Canadian Nuclear Laboratory (CNL)
- The High-Performance Research Computing (HPRC) center at Texas A&M University provided the computational resources needed for this work

Mechanical Loading

- The choice of loading state reduced chances of hardening and thereby promote 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



- Mechanical responses of GB models with and without inclusion are qualitatively similar

Conclusions: what about cracks?

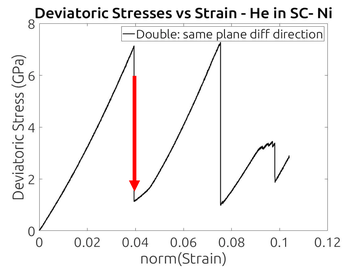
- No crack is observed at slip bands forming in our model
- Next step: slip vector and bubble analysis on all large models

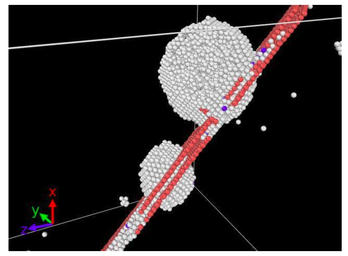
High performance computing summary

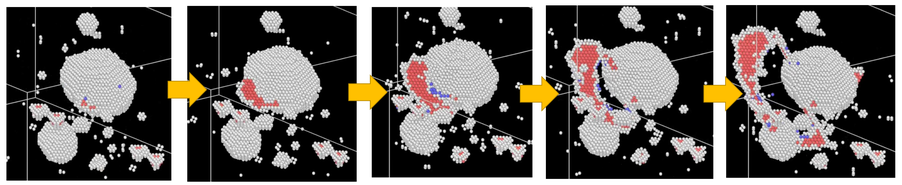
- Implemented using LAMMPS on ADA and TERRA at HPRC
  - Small 100K-atoms: 320 cores, 2.5G memory ~48 hrs (ADA)
  - Large 10M-atoms: 512 cores(GPU nodes), 8G memory for ~1224 hrs (TERRA)

Shearing of He bubbles

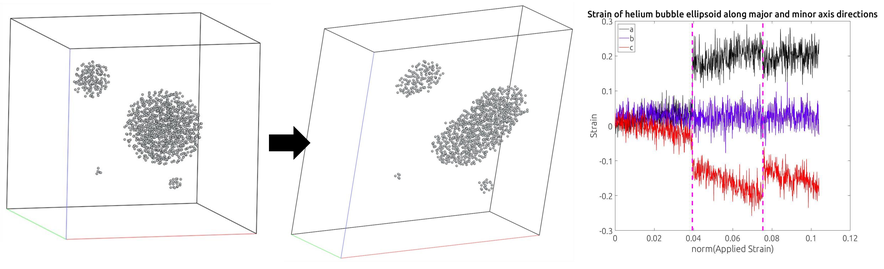
Dislocations cut through bubbles during stress drops





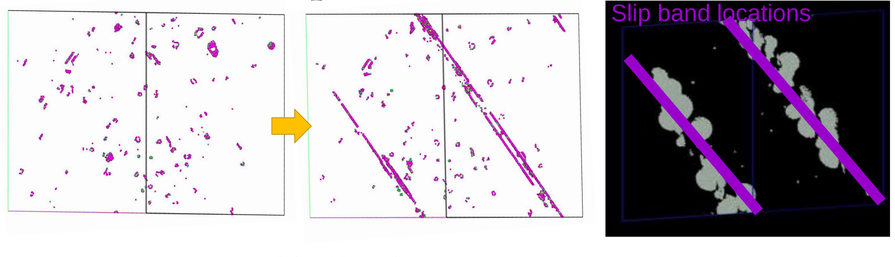


Dislocation impart permanent shape change to He bubbles



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

Slip Band Formation



Large model: ~10M Ni atoms, ~47 nm x 47 nm x 47 nm

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