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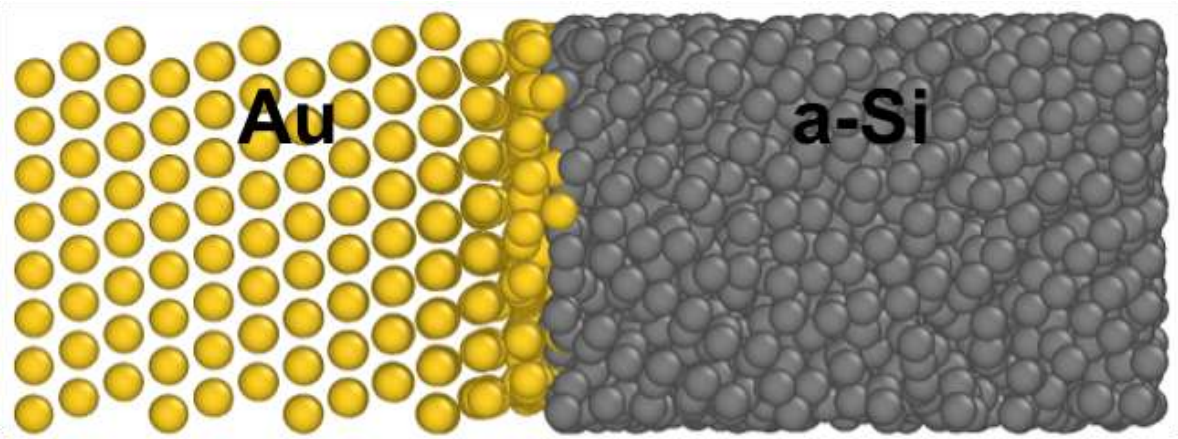
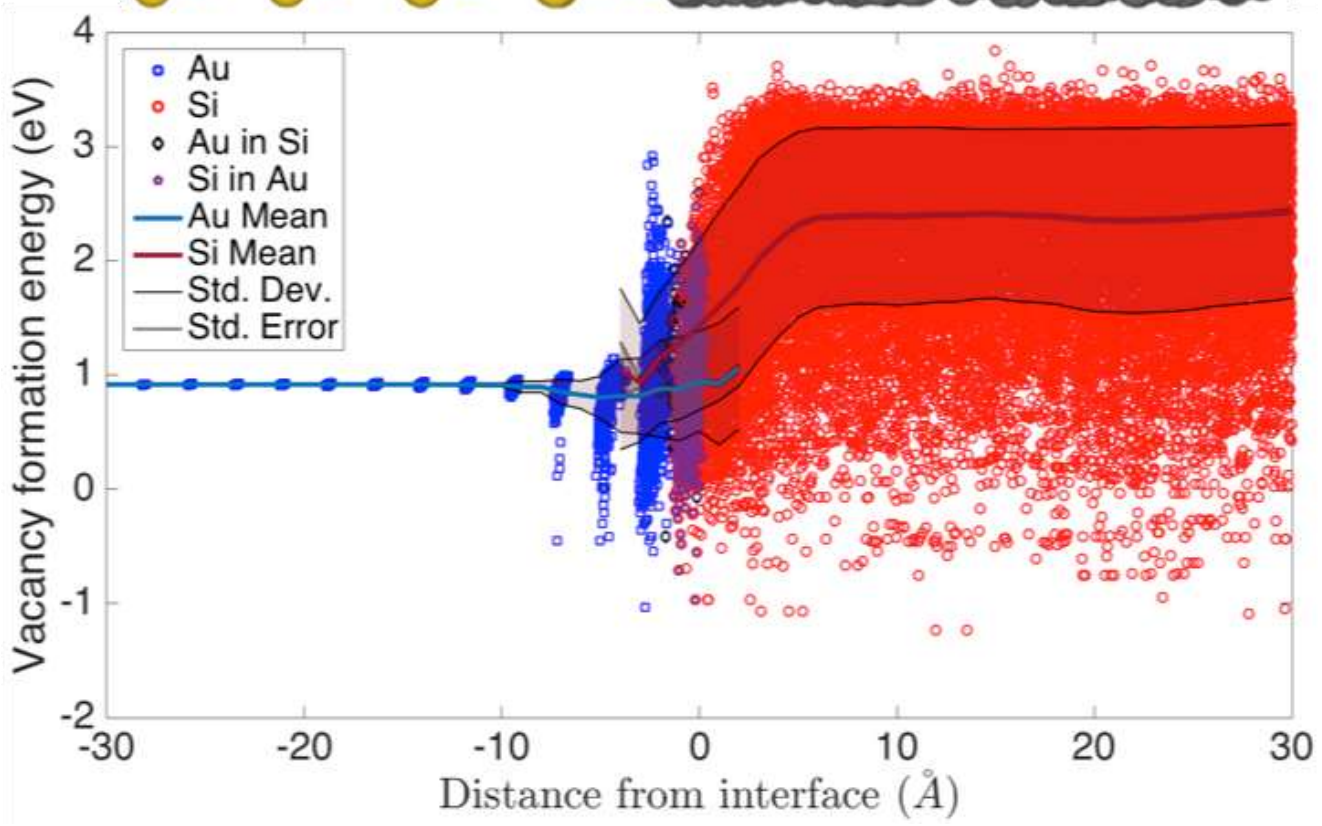
Supercomputing Conference

Nov. 2018

Formation energies of vacancies in Au/a-Si model

- 6 Au/a-Si models
- ~100,000 vacancies near interface per model





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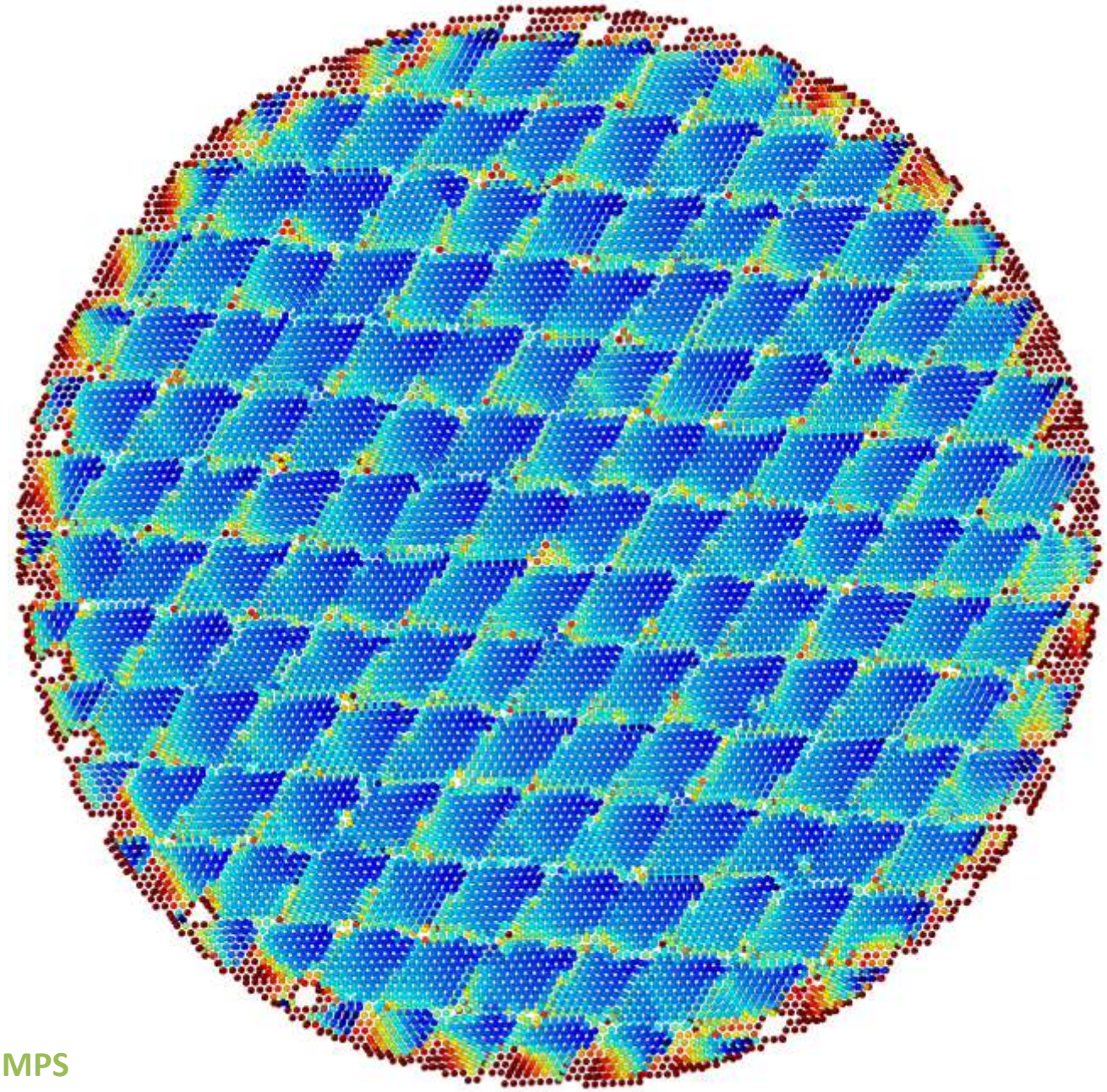
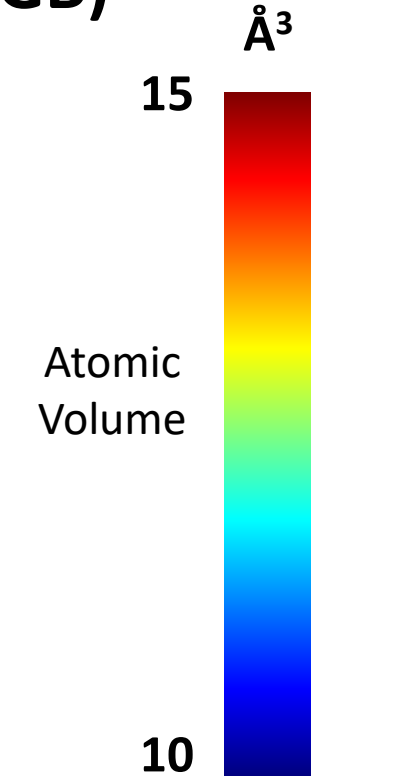
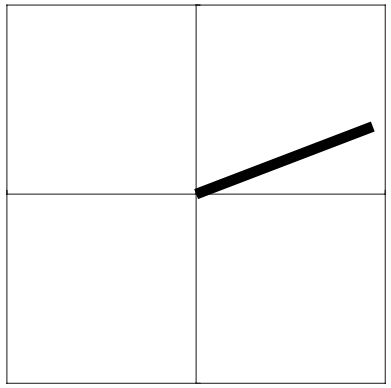
LAMMPS Fortran 90 Matlab Bash

Internal structure of Ni grain boundary (GB)







Crack propagation direction

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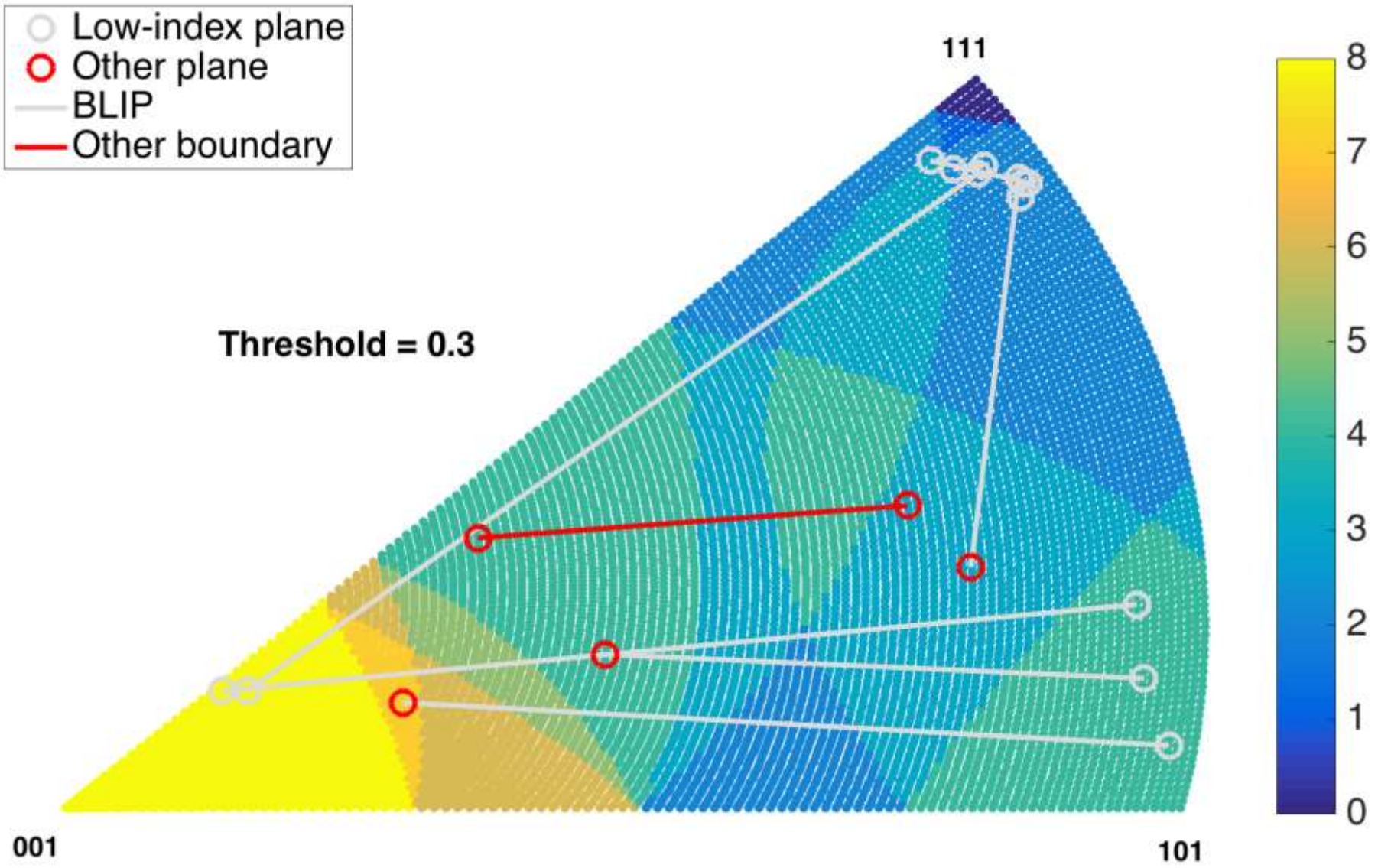
Schmid factor analysis for crack resistant Ni GBs



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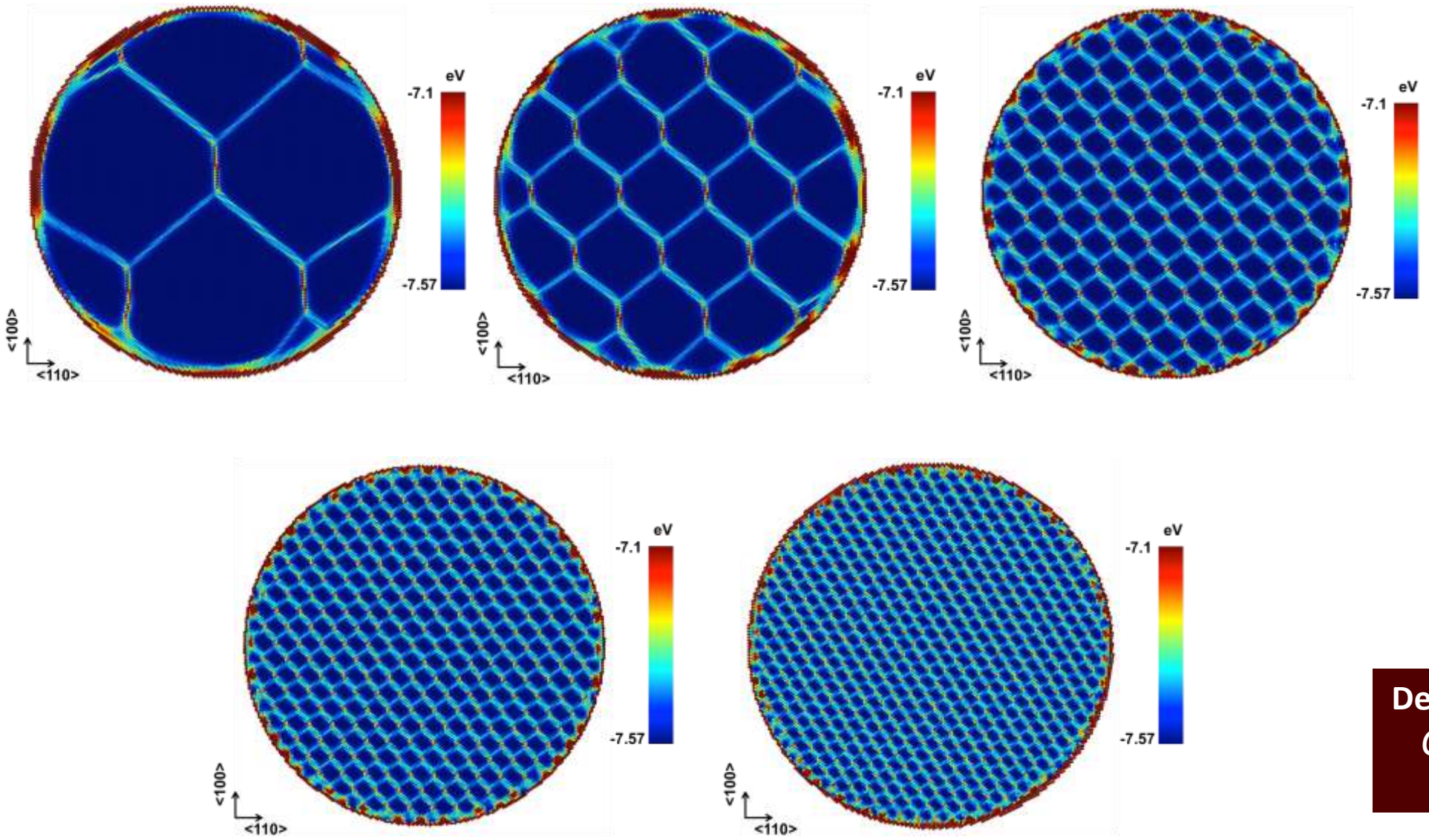
Matlab

Analyzing dislocation structures at Nb twist GBs



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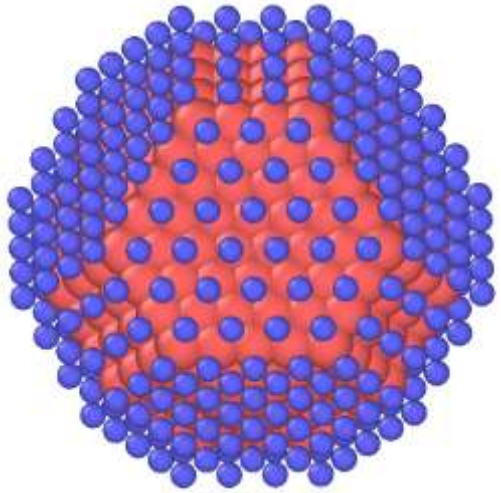
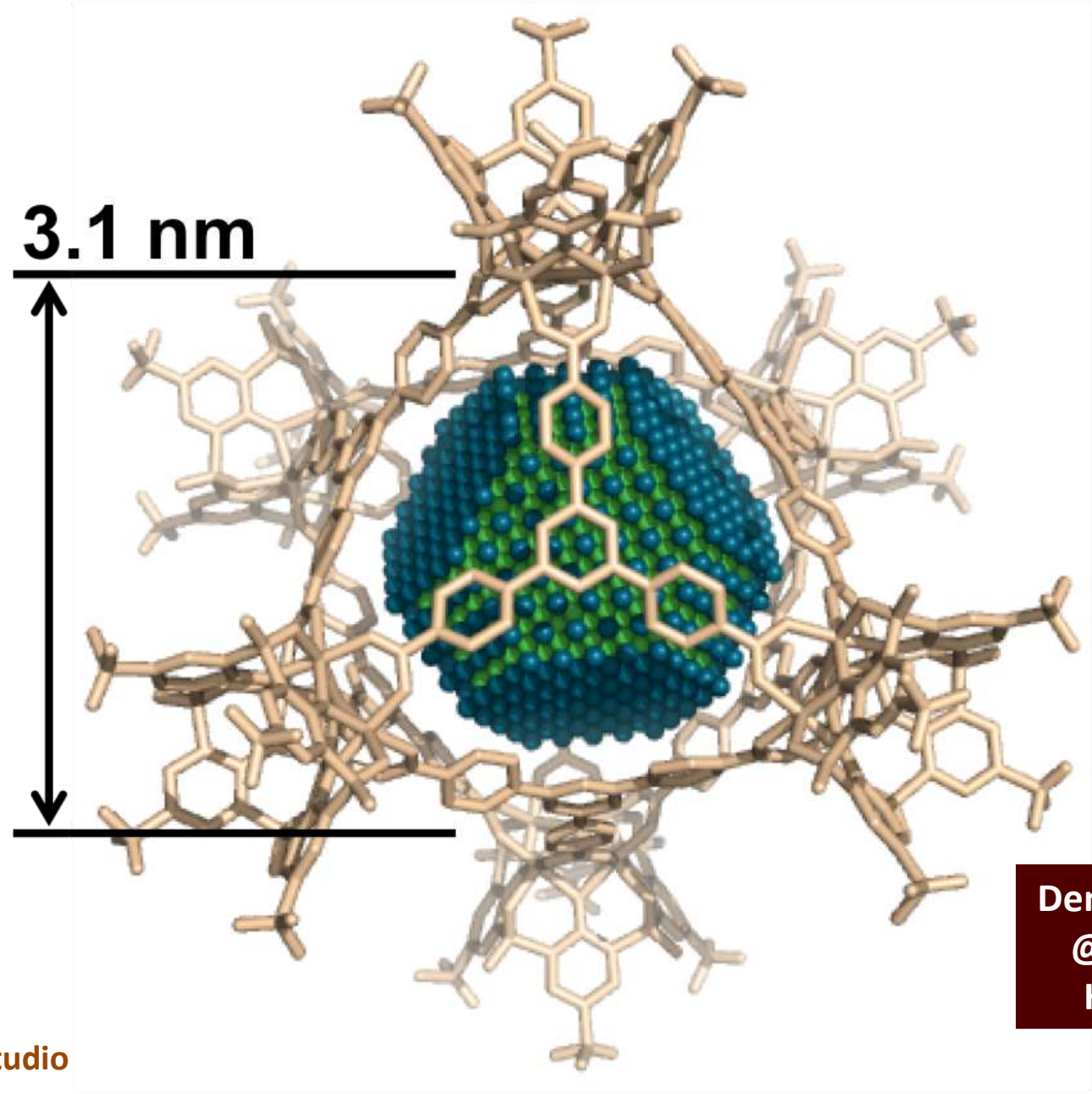
Ni/Pd core/shell nanoparticle in Metal-organic Frameworks (MOFs)



Ni (core) – Pd (shell) particle



LAMMPS Matlab Materials Studio

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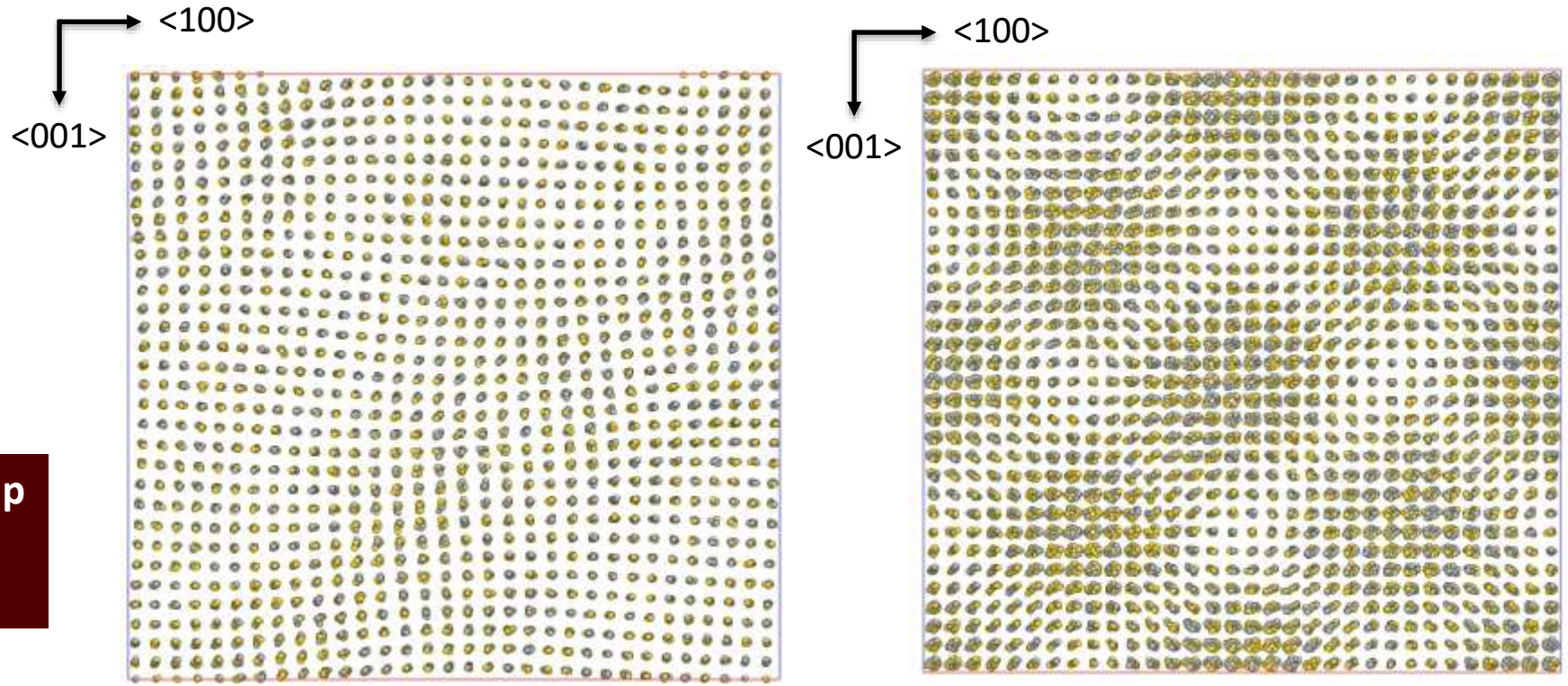
Cyclic loading on Model Equiatomic Solid Solutions (ESSs)

- Model: Two component, defect-free, face-centered cubic ESSs
- “Resonance” patterns observed after 40-150 cycles of loading at specific strain rates and temperatures



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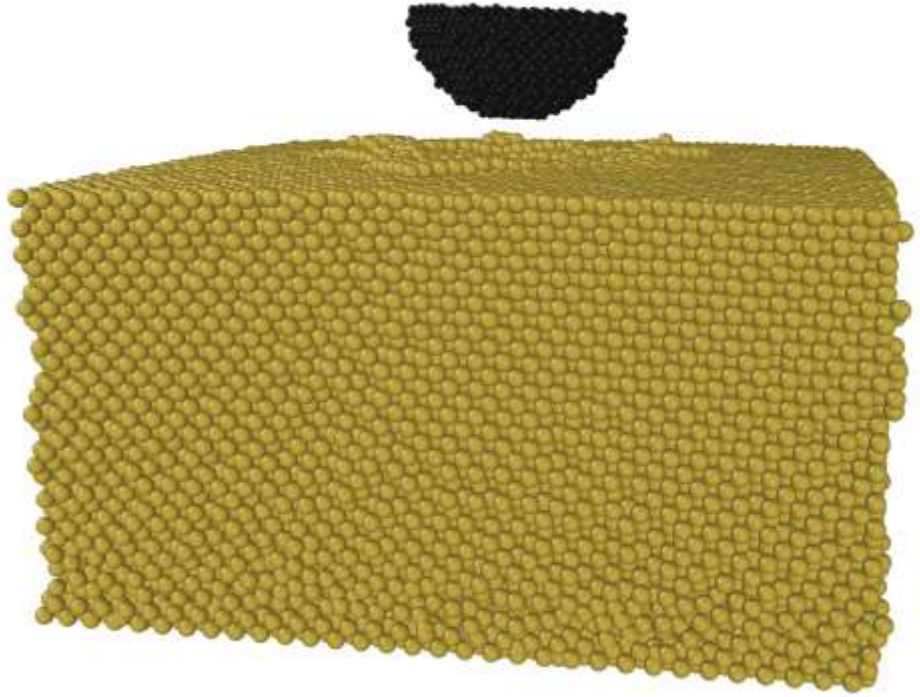
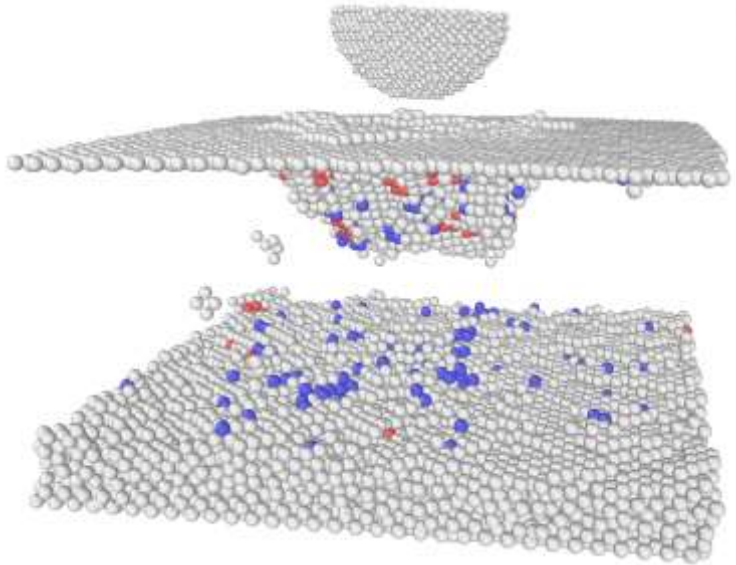
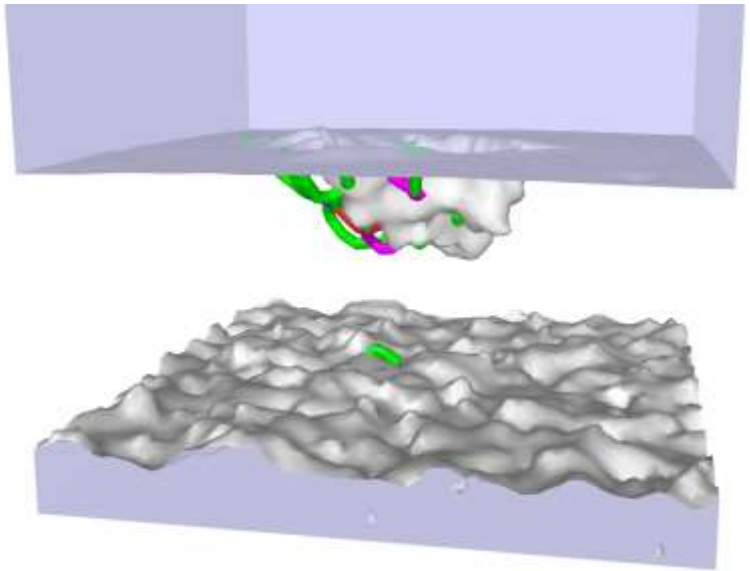
Nano-indentation of single crystal copper (Cu)

Simulation setup



Common neighbor analysis





Dislocation extraction algorithm

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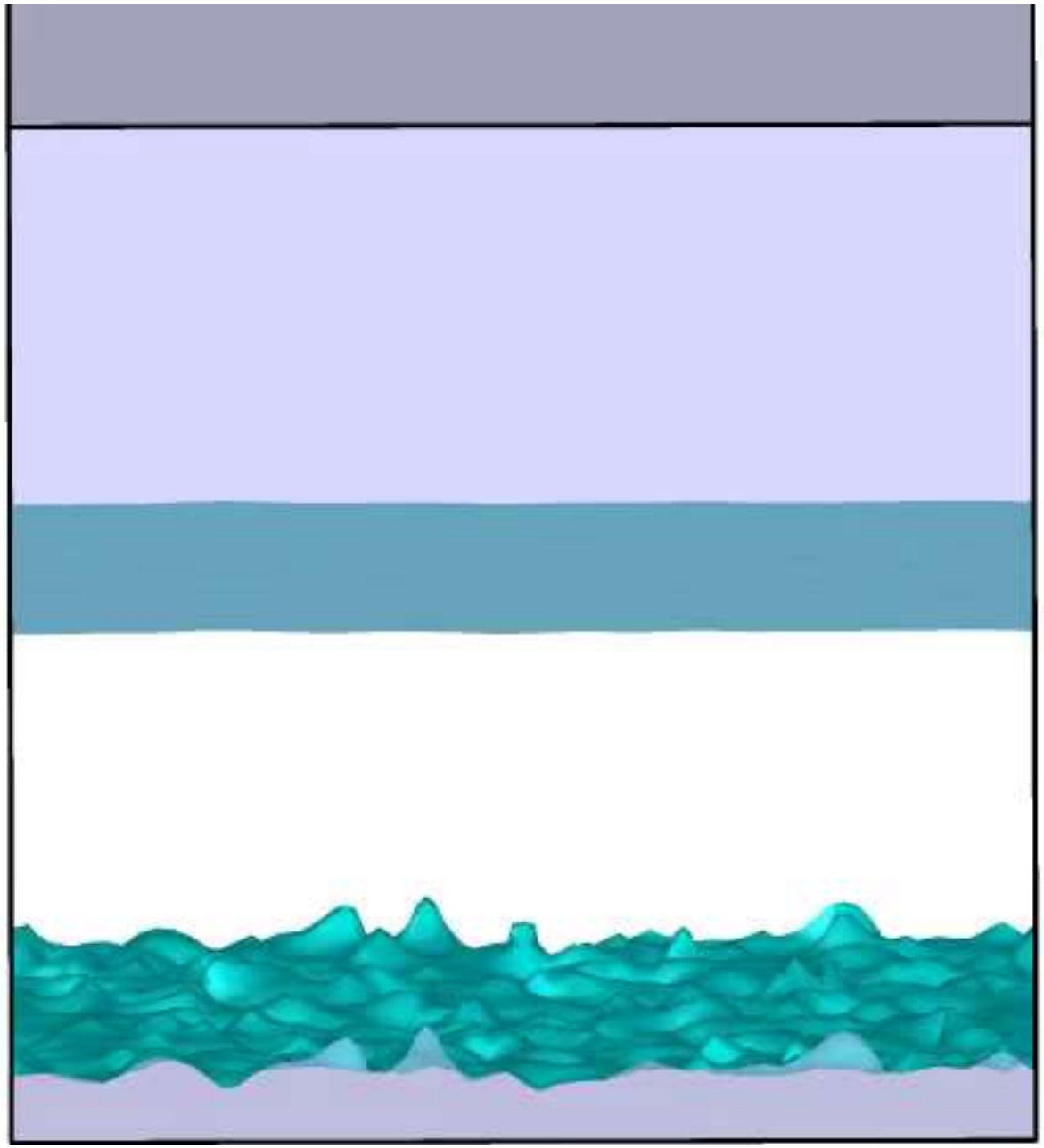
Nano-indentation of Cu - video



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