Molecular dynamics simulation of high strain rate nanoindentation

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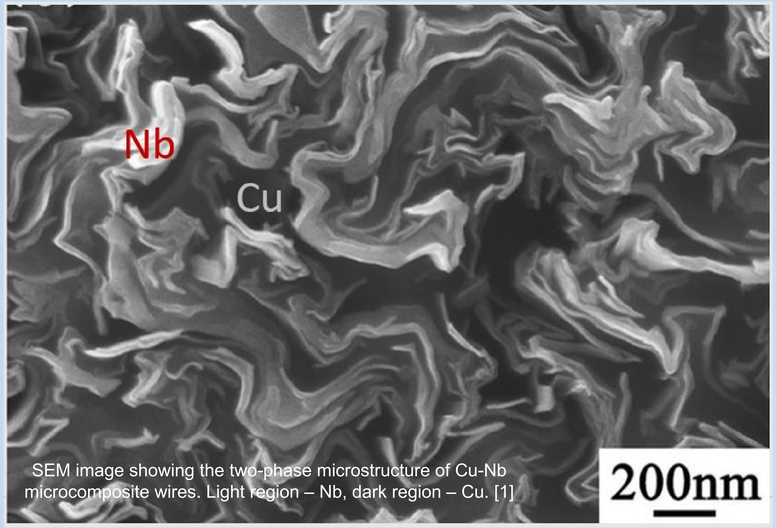
CREDDS
Center for Research Excellence on Dynamically Deformed Solids

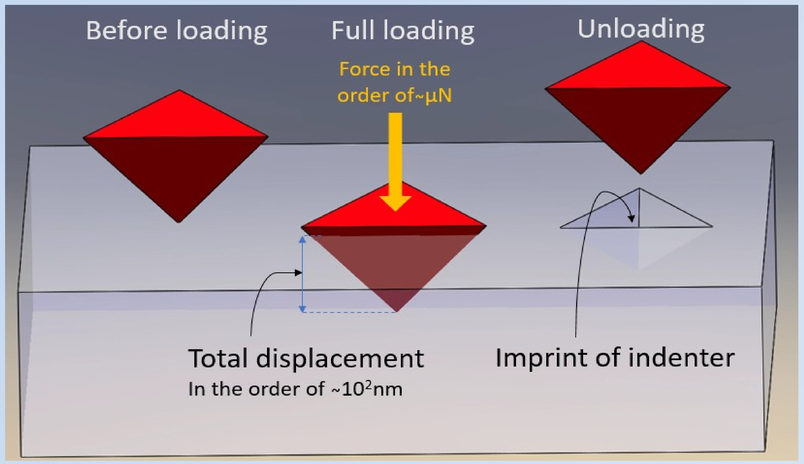
Deformation of heterogeneous materials

Multiphase materials deform differently under high strain rates compared single-phase polycrystalline solids.



SEM image showing the two-phase microstructure of Cu-Nb microcomposite wires. Light region – Nb, dark region – Cu. [1]

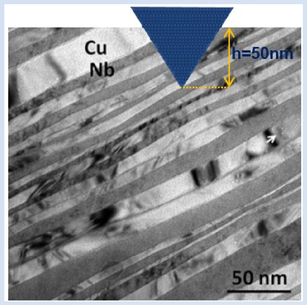
Nanoindentation - a powerful technique for probing local heterogeneity



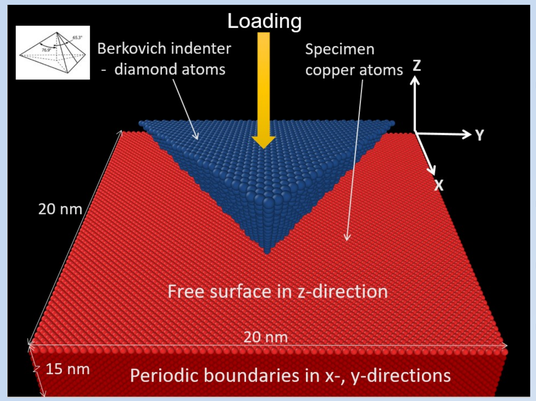
CREDDS is developing a high strain rate (10^5– 10^6 s^{-1}) nanoindentation system under the leadership of Dr. George M. Pharr (TAMU)

Molecular dynamics (MD) simulations can match the length- and time-scales of nanoindentation experiments

- Sample size ~ 300 x 300 x 150 nm, containing ~1.1 billion atoms,
- Displacement 50nm, initial velocity 100m/s
- A 1 month allocation at a leadership-class computing facility would be required



Simulation of nanoindentation

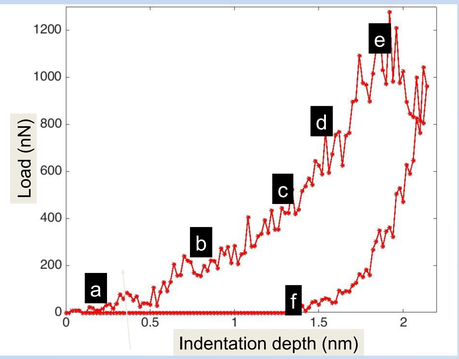


A computational sample, simulated with LAMMPS [3], visualized with OVITO [4].

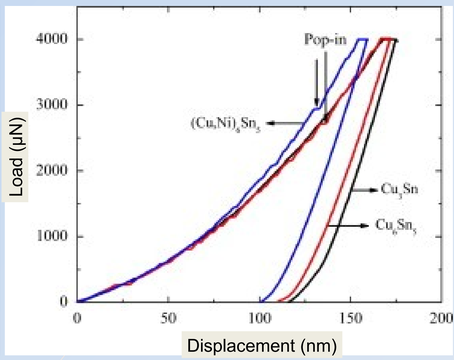
- Parallel simulations using LAMMPS
- Hybrid potentials (LCBOP, EAM, Lennard Jones)
- Room temperature
- NVE emsemble
- TAMU's high performance research computing (HPRC) program

Load - displacement relationship

Displacement response to applied load can be investigated by both simulation and experiment

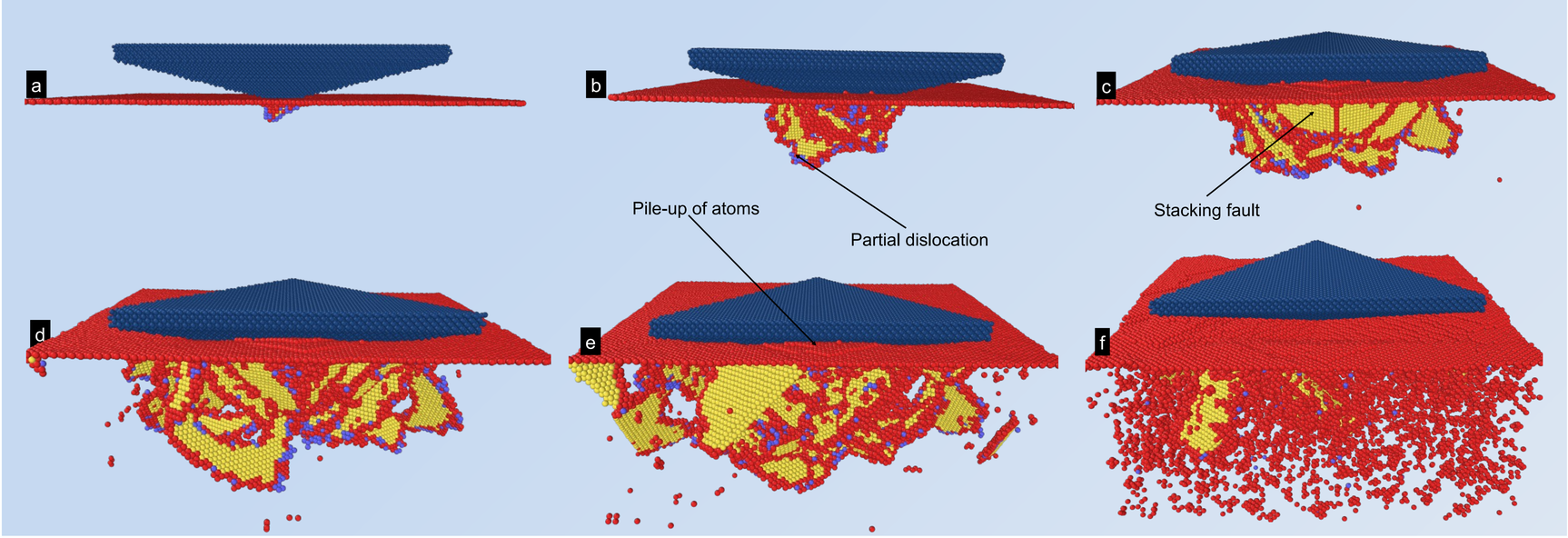


MD load-displacement curves have a similar form to experimental nanoindentation. a-f: different stages of indentation



Illustrative experimental load-displacement curves of intermetallic compounds [5]

Subsurface deformation evolution revealed by MD



Acknowledgments and references

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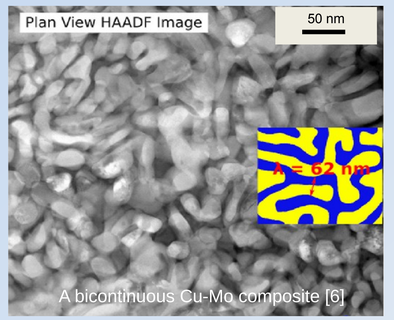
References:

[1] L. Deng, J. Mater. Sci. (2019), 54:840-850.
[2] I. J. Beyerleina et al., Proc Natl Acad Sci. 2014;111(12):4386–4390
[3] S. Plimpton, J Comp Phys, 117, 1-19 (1995).
[4] A. Stukowski, Modelling Simul. Mater. Sci. Eng. 18 (2010).
[5] A. Rahman et al., Mater. letters 147 (2015) 50-53.
[6] Y. Cui et al., Materials and Design 166 (2019) 107602.

Research direction

- Replicate PVD multiphase materials made in the group of Dr. A. Misra, University of Michigan, Co-PI of CREDDS.
- Collaborate with nanoindentation group to elucidate the role of interfaces in high strain rate deformation response.
- Using two-temperature model to accurate model dissipation of heat generated during deformation



A bicontinuous Cu-Mo composite [6]