Novel Methods for Phase-Transformation-Assisted Twinning in Molybdenum Nanomaterials

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1. Project Objectives and Goals

- ❑ Enhance ductility and strength in bcc Molybdenum (Mo) nanomaterials.
- ❑ Investigate deformation mechanisms across various Mo nanowires (NWs) and bulk Mo structures under uniaxial tension and compression.
- ❑ Elucidate the role of crystal orientations on deformation mechanisms (e.g., twins or slips).

2. Background & Motivation

- ❑ Twin can improve strength (via dislocation pile-ups) and ductility (via activating new planes for dislocation motions).
- ❑ Twinning in bcc materials (e.g., Mo) is less frequently observed due to high energy barrier.
- ❑ Phase transformation (PT) can act as a potential stress-induced twin formation route.
- ❑ How? Utilizing high-stress to trigger PT-assisted twinning, as shown in a study with a nano-porous Cu/Mo structure.[1]
- ❑ Nanowires ✓, pre-cracked bulk samples ✓, Cu/Mo interfaces, texturized polycrystals, and nano-porous structures can be utilized for triggering PT-induced twins.

3. Methods

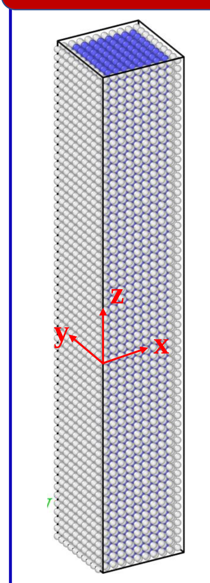
Mo Nanowires:

- ❑ Molecular Dynamics (MD): LAMMPS
- ❑ Density Functional Theory (DFT): Quantum Espresso
- ❑ Pre-/Post-Process: OVITO, MATLAB, Python

Cu/Mo interfaces:

- ❑ Experimental: Magnetron co-sputtering, STEM, HRTEM,

4. Structures



Case	x	y	z
1	[100]	[010]	[001]
2	[110]	[$\bar{1}$10]	[001]
3	[11$\bar{2}$]	[111]	[1$\bar{1}$0]
4	[1$\bar{1}$0]	[11$\bar{2}$]	[111]

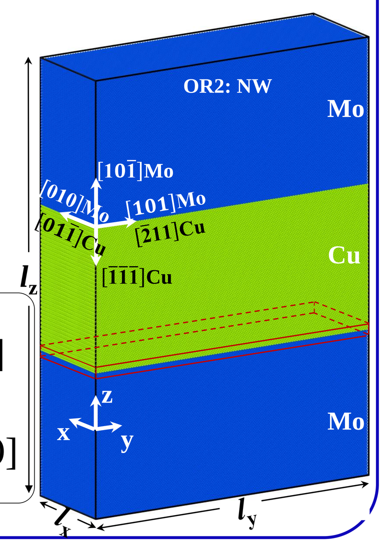
Orientation Relationships:

GT: Greninger-Troiano

NW: Nishiyama-Wassermann

OR1: GT: Cu(111)[1$\bar{2}$1] || Mo(011)[01$\bar{1}$]

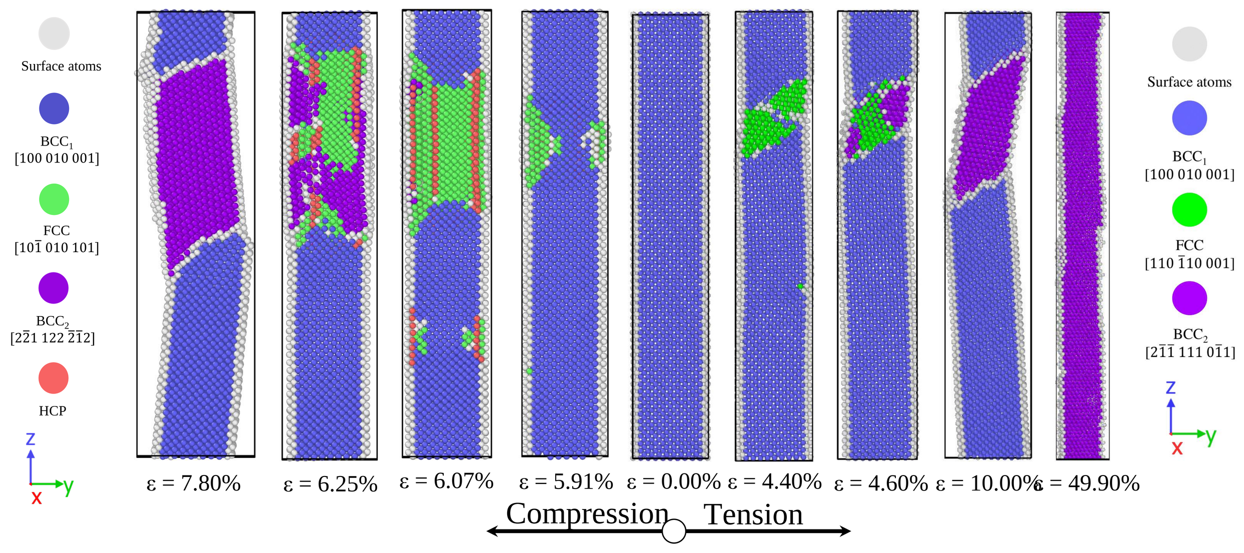
OR2: NW: Cu(111)[01$\bar{1}$] || Mo(10$\bar{1}$)[010]



5. Results

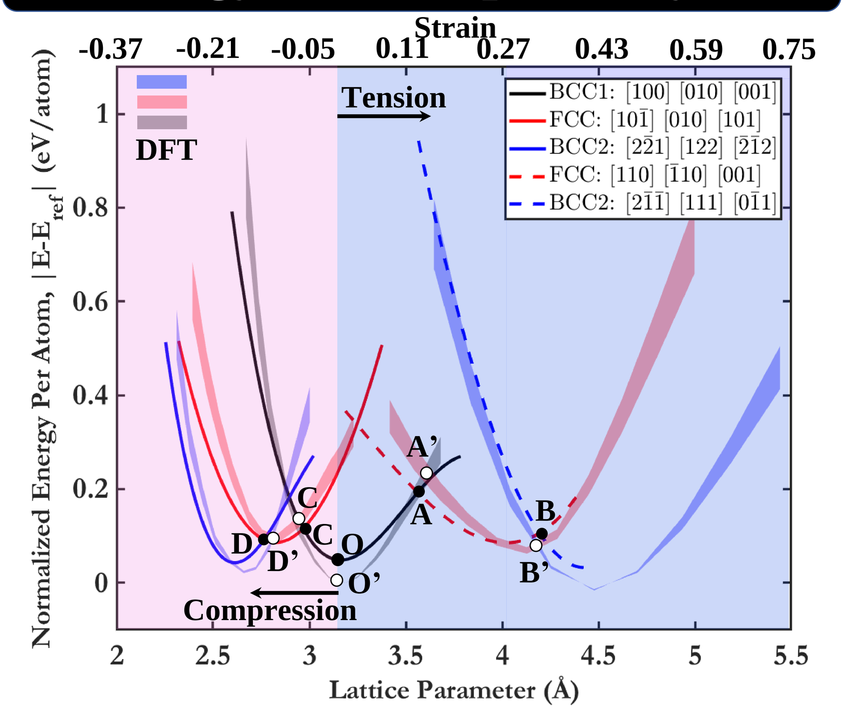
5.1 Response of Mo Nanowires (NWs) to Deformation

Phase Transformation (PT)

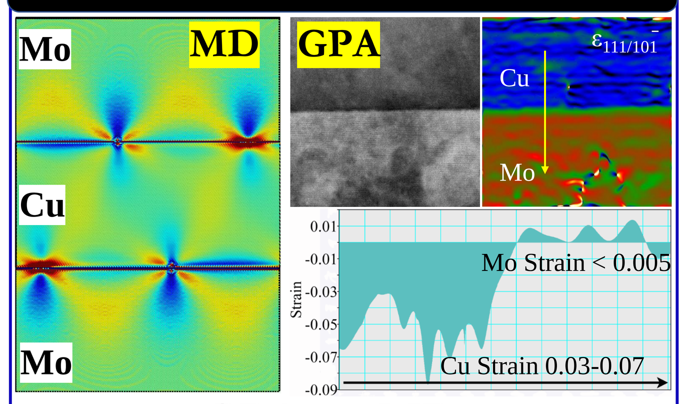


❑ BCC_1 $\xrightarrow[\text{Bain}]{\text{PT}}$ FCC $\xrightarrow[\text{Pitsch}(t)/\text{Bain}(c)]{\text{Twin}}$ BCC_2 [2]

Energy Landscape Analysis



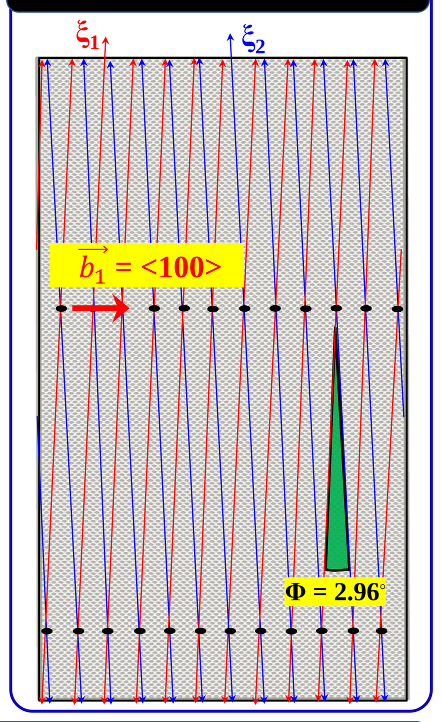
Elastic Strain Distribution



GPA vs. MD

Method	ε_z in Cu	ε_z in Mo
GPA	~0.06	~0.005
MD	~0.062	~0.006

Misfit Dislocation



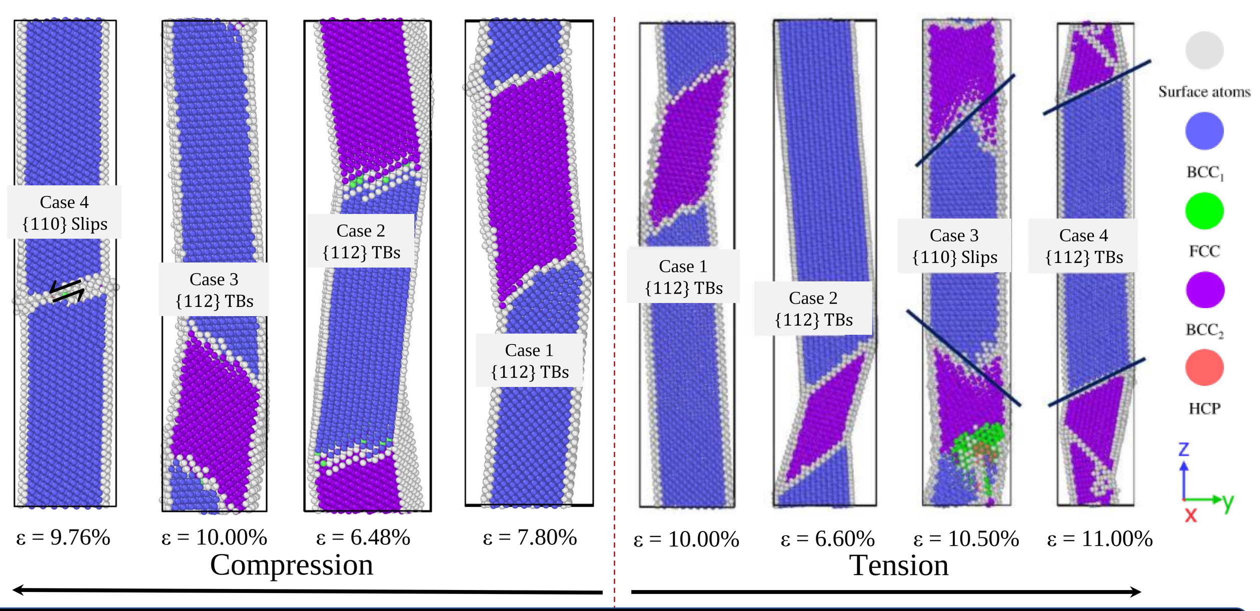
Deformation Mechanisms in 4 Mo Nanowires

Tension:

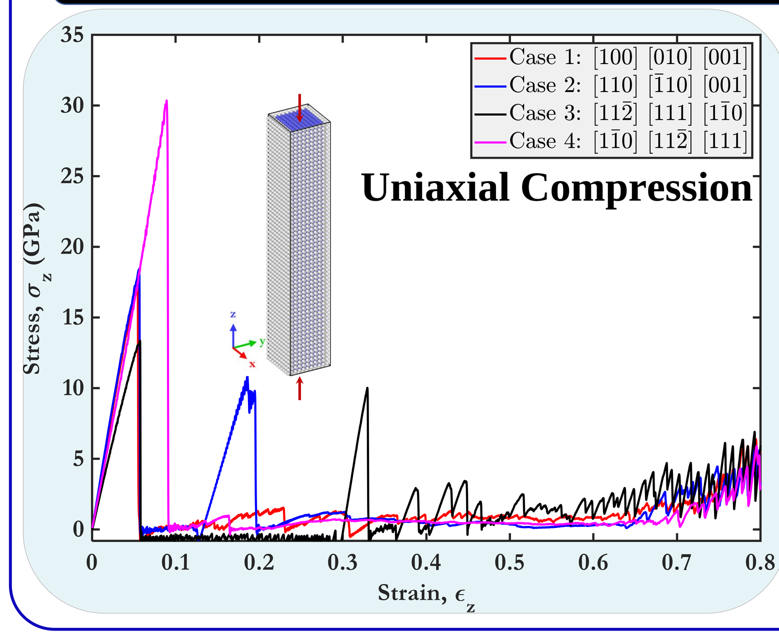
- ❑ **Cases 1 & 2** = PT + {112} Twins
- ❑ **Case 3** ={110} Slips
- ❑ **Case 4** = Classical Twins

Compression:

- ❑ **Cases 1, 2, & 3** = PT + {112} Twins
- ❑ **Case 4** = {110} Slips



Stress-Strain Profiles

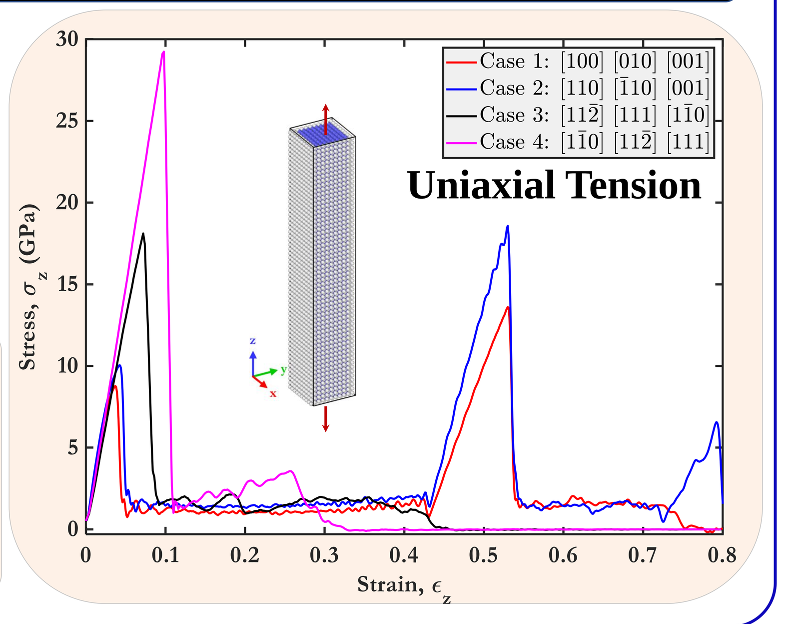


Compression:

- ❑ **Case 1**: less ductile
- ❑ **Cases 2 & 3**: Secondary elasticity
- ❑ **Case 4** : brittle, strongest

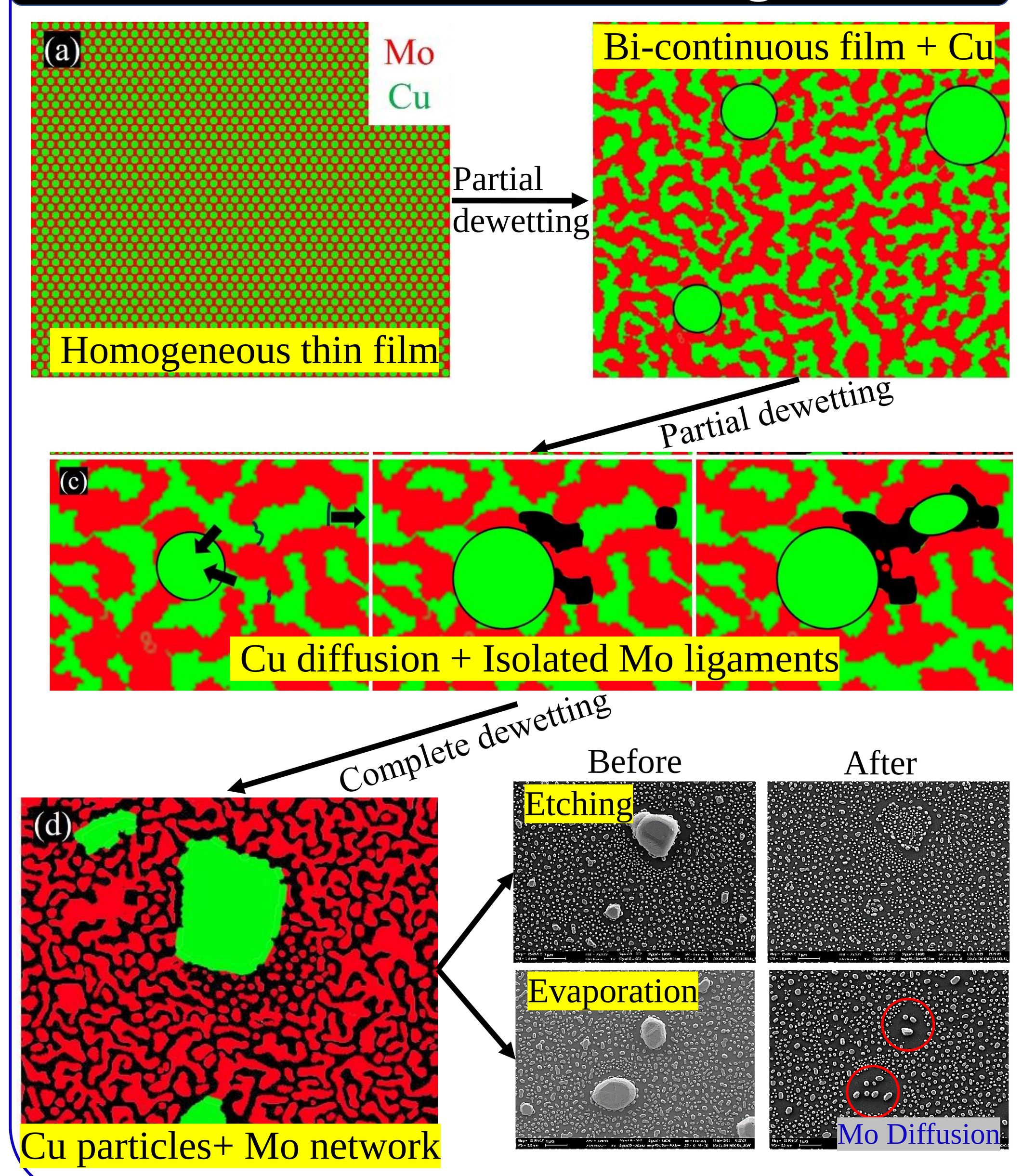
Tension:

- ❑ **Cases 1 & 2:** Secondary elasticity
- ❑ **Case 3:** less ductile
- ❑ **Case 4:** brittle but strongest



5.2 Cu/Mo Semi-Coherent Interfaces

Solid-State De-wetting



Kinetic/Diffusion Model

Initially: $V_{Cu} < V_{Mo}$

Diffusion halts: $V_{Cu} = V_{Mo}$

Diffusion Flux, $J \approx \frac{D_e \delta \Omega \Delta\gamma}{k_B T r^2}$

$V_{Mo} \approx \nabla \cdot J$

$V_{Mo} = V_{Cu} \approx \frac{D_e \delta \Omega \Delta\gamma}{k_B T r^3}$

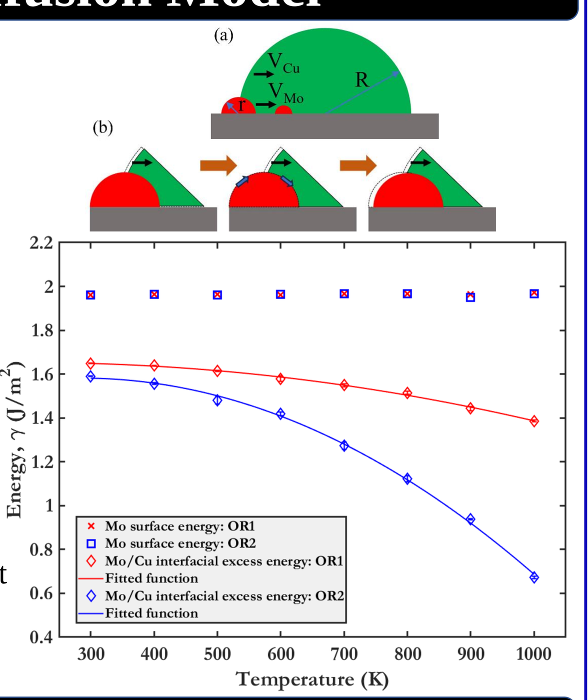
D_e = 4.53e-13 m^2/s

≈ 4.21e-14 m^2/s [3]

D_e: Surface/interface diffusion coefficient

δ: Width of the surface layer (~0.5 nm)

Ω: Atomic volume of Mo



Possibility of Drag/Friction

Assumption: The critical size of agglomerated Mo is **NOT** influenced by direct mechanical drag between Mo and sapphire substrate.

Tune EAM to modify interactions → Stop when $\Gamma_{MD} = \Gamma_{exp}$ → Get τ_{int} → $r_{max} = \frac{\Delta\gamma}{\tau_{int}}$, $\Delta\gamma = \gamma_{Mo} - \gamma_{Mo/Cu}$ → compare → r_{exp} ~134 nm

$r_{max} \neq r_{exp}$

Mo agglomeration is not affected by drag

6. Conclusion

- ❑ Crystal orientation plays a major role in activating deformation mechanisms (slips/twins) in bcc Mo NWs
- ❑ PT-assisted twins are achieved in certain Mo NWs under certain loading conditions
- ❑ Cu/Mo interfacial stress may potentially help achieve PT-assisted twins under deformation

7. Future Studies

- ❑ Extrapolate to Cu/Mo interfaces, Mo polycrystals with random/texturized grains, and nanoporous Mo structures.

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- **Center for Integrated Research Computing** (CIRC), University of Rochester
- **Advanced Computational Mechanics and Materials Laboratory** (ACMML), University of Rochester

9. Publications

1) A. Mostafa, L. Vu, Z. Guo, A. K. Shargh, A. Dey, H. Askari, and N. Abdolrahim. "Phase-transformation assisted twinning in Molybdenum nanowires." *Comput. Mater. Sci.* 244 (2024): 113273.
2) F. Li, A. Mostafa, J. Zimmerman, Z. Liang, L. Klinger, J. Yeom, J. Janczak-Rusch, N. Abdolrahim, E. Rabkin, "Solid-state dewetting of co-sputtered thin Mo-Cu films accompanied by phase separation," 2024 (Under Preparation).

10. References

1. L. He and N. Abdolrahim. "Stress-assisted structural phase transformation enhances ductility in Mo/Cu bicontinuous intertwined composites." *ACS Appl. Nano Mater.* 2.4 (2019): 1890-1897.
2. A. Mostafa, L. Vu, Z. Guo, A. K. Shargh, A. Dey, H. Askari, and N. Abdolrahim. "Phase-transformation assisted twinning in Molybdenum nanowires." *Comput. Mater. Sci.* 244 (2024): 113273.
3. B.C. Allen, The surface self-diffusion of Mo, Cb (Nb), and Re, *Metallurgical Transactions* 3 (1972) 2544–2547.