Phase transition mechanism in Molybdenum nanowires

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INTRODUCTION

In metallurgy study, finding the crystallographic orientations to enhance the strength and ductility of the materials under the loading has been a huge interest. Molybdenum (Mo), a metal with high melting point and stiffness, has not been well studied compared to other common metals such as Copper, Steel, etc. This research studies the higher ductility observed in Mo nanowires under specific lattice orientations. This phenomenon has been observed before [1,2]. However, the specific reasonings behind the phase transition and orientation transformation have not been answered thoroughly.

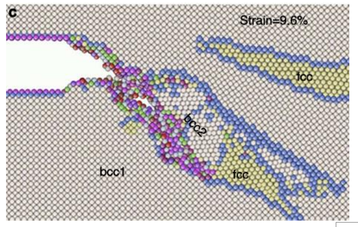

Figure 1: Phase transition observed in Mo structure [1]

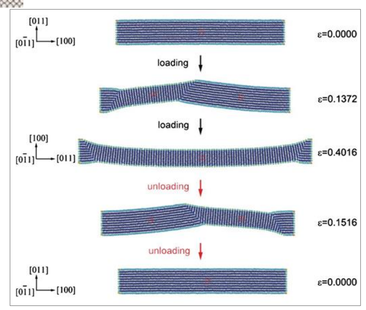

Figure 2: Orientation transformation in Mo nanowire [2]

Objectives:

1. Simulate Mo nanowires using molecular dynamics (MD) computational methods and observe the structures' deformation mechanisms.
2. Identify specific lattice orientations which enhance the nanowires' ductility.
3. Explain the phase transition and orientation transformation happening under specific lattice orientations and allowing the nanowires undergo a much larger strain range.

COMPUTATIONAL METHODS

- Four Mo nanowires are constructed using LAMMPS* code with the size of 3nm x 3nm x 19nm [3].
- The inter-atomistic potential used to create the nanowires is CuMo.eam [4,5].
- All nanowires are loaded under the same conditions of temperature (300K) and uniaxial loading (along Z direction). Stress-strain curves are plotted using MATLAB.
- Ovito visualization is utilized to observe the deformation mechanisms [6].

	X	Y	Z
Case 1	[100]	[010]	[001]
Case 2	[110]	[$\bar{1}$10]	[001]
Case 3	[11$\bar{2}$]	[111]	[1$\bar{1}$0]
Case 4	[1$\bar{1}$0]	[11$\bar{2}$]	[111]

Table 1: Lattice orientations in four nanowires (written in Miller index form [hkl]).

** Large-scale Atomic/Molecular Massively Parallel Simulator code*

RESULTS

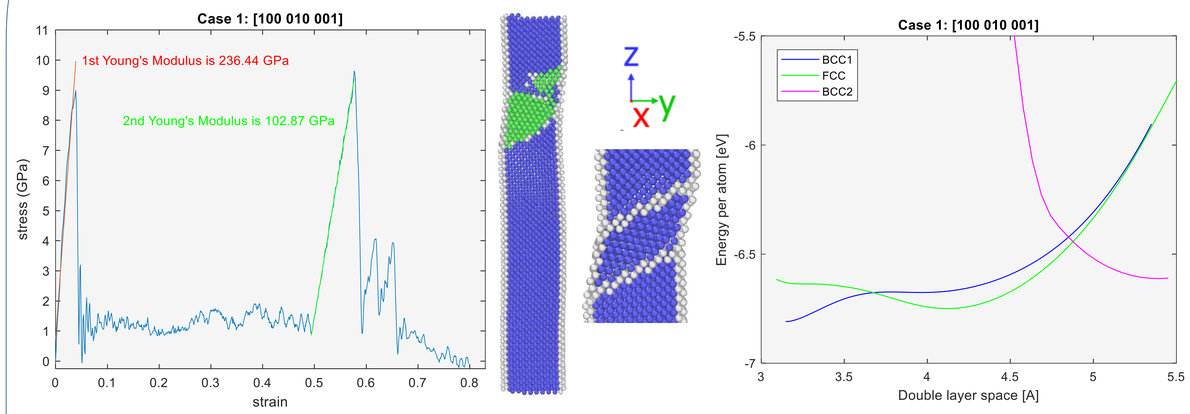

Figure 3 – Case 1: (a) Stress-strain curve, (b) fcc at 4.5% strain (Ovito), (c) Twin boundaries formation on {112} at 4.6% strain, (d) Energy curve

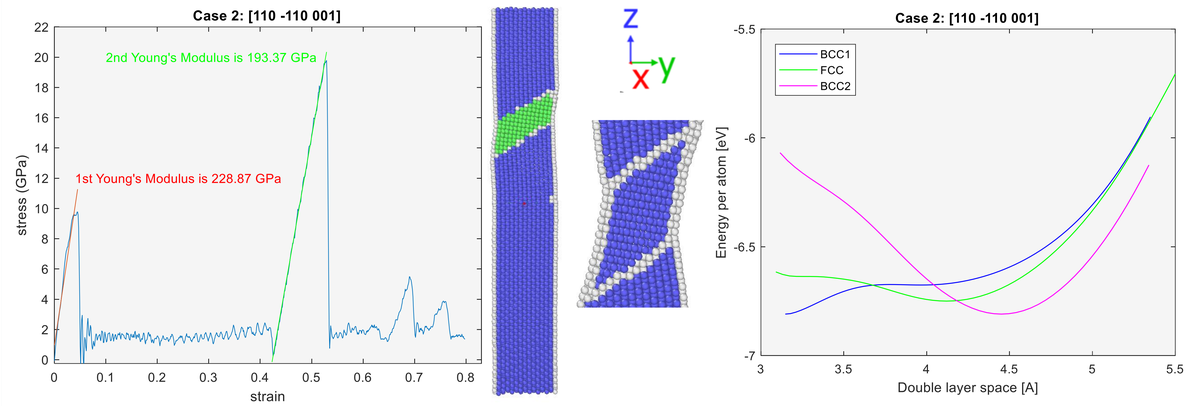

Figure 4 – Case 2: (a) Stress-strain curve, (b) fcc at 4.9% strain (Ovito), (c) Twin boundaries formation on {112} at 5.2% strain, (d) Energy curve

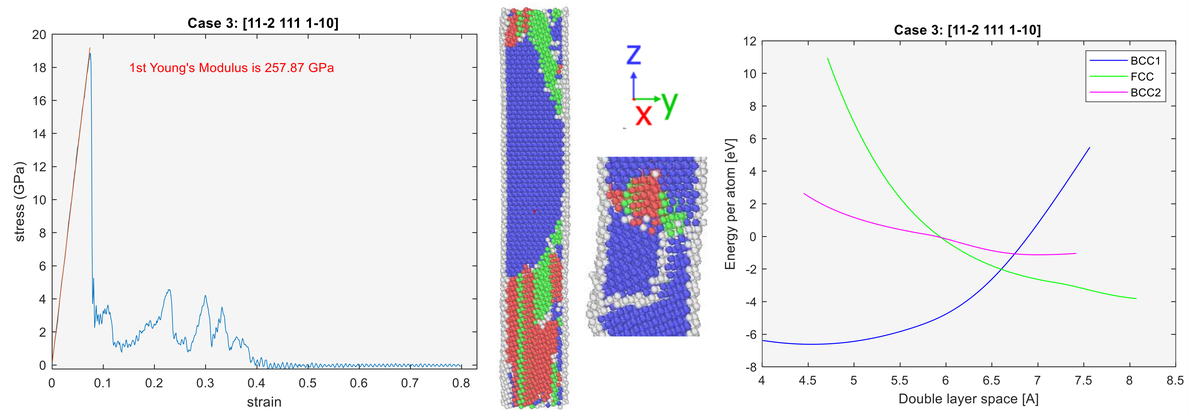

Figure 5 – Case 3: (a) Stress-strain curve, (b) fcc at 7.9% strain (Ovito), (c) No twin boundaries formation (9.2% strain), (d) Energy curve

DISCUSSION

- The energy curves confirm that bcc1-fcc-bcc2 phase transition only occur in Case 1 and 2 (loading direction Z of [001]).
- The twin boundaries (TBs) only form in Case 1 and 2 and appear right after fcc atoms disappear. The TBs plane in both cases is {112} which agrees with previous work [2].
- The TBs formation is followed by the TBs propagation throughout the whole nanowire. This TBs propagation transforms the structure orientation completely from bcc1 to bcc2.
- The transformed structure of bcc2 undergoes a second elastic region which gives a higher second yield strength.

CONCLUSION & ONGOING RESEARCH

Conclusion

- The phase transition bcc1-fcc-bcc2 and orientation transformation are orientation dependent (only occur in [001] loading direction).
- This is an optimal condition since the transformed structure undergoes a second elastic region, reaches a higher second yield strength, and undergoes a larger strain range of 100%.

Ongoing research

- Explain why the TBs form following the phase transition only in Case 1 and 2 (loading in [001])
  - Why slipping plane {112} is activated after fcc atoms
  - How this TBs plane {112} connects fcc with bcc2.
- Explain why Case 2 nanowire reaches a much higher second yield stress than Case 1

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