Deformation mechanisms and pseudoelastic behaviors in trilayer composite metal nanowires

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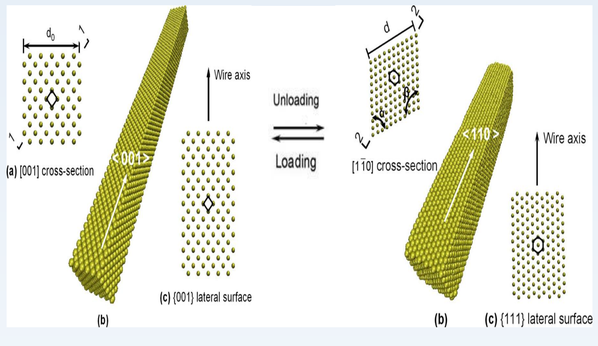
Background

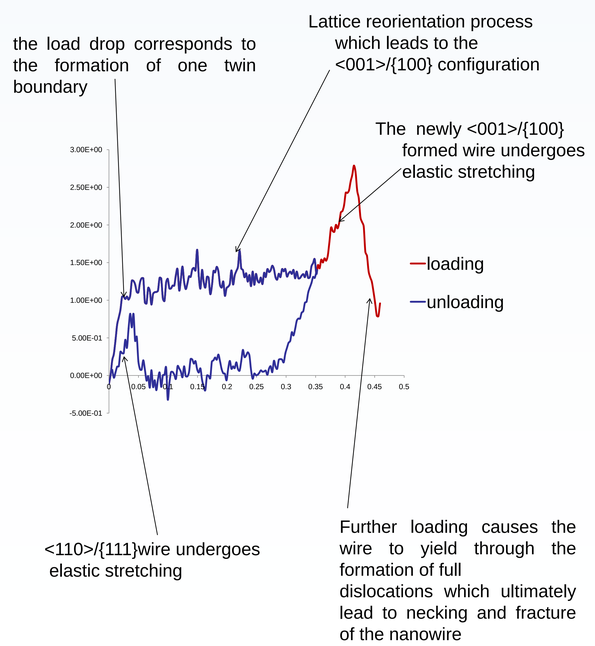
Nanowires are typically single-crystalline, highly anisotropic nanostructures that result from rapid growth along one direction.
defect-free fcc single crystalline nanowires can completely recover from severe deformations, up to 50% strains, well beyond the recoverable strains of 5-8% typical for most bulk shape memory alloys



Cu nanowire before relaxation:
a) {001}square lattice
on square cross sections; b) external view of the nanowire; c) {001}square lattice on lateral surfaces

The reconstructded Cu nanowire after relaxation: a) [110] elongated hexagonal lattice on a rhombic cross section; b) external view of the reconstructed nanowire; c) {111}square lattice on lateral surfaces

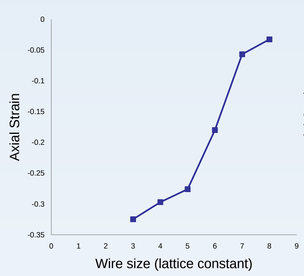
The stress-strain curve of a reconstructed CU nanowire with the size of 1.8x1.8nm at 300 K



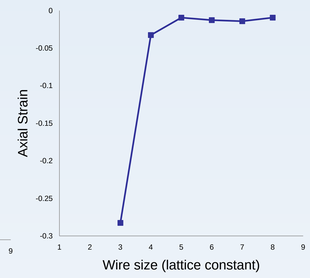
Objectives

Critical size of exhibiting pseudoelasticity in Cu & Ni nanowires

The critical size of showing pseudoelasticity is 2.19x2.19nm for Cu Nanowires at 300K



The critical size of showing pseudoelasticity is 1.6x1.6nm for Ni nanowires at 300K



1)Increasing the critical size of showing pesudoelastic behavior by:

➢Development of a strong interface between the layers with high coherency stress due to the lattice misfit between two layers

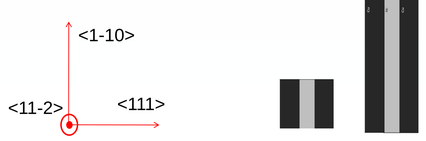
2) Comparison of the yield points between the Cu nanowires and composite nanowires

Methods

✓completely coherent interfaces with the coherent strains of :

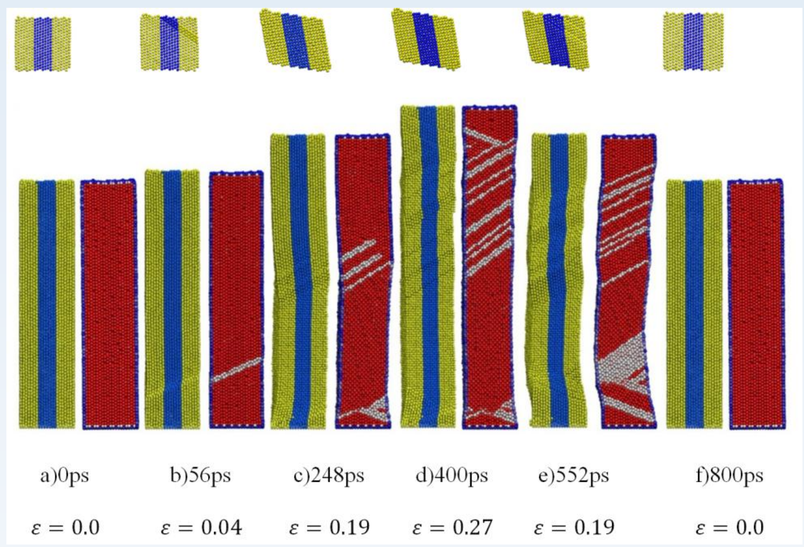
$$Cu \quad \begin{cases} \varepsilon_{11} = \varepsilon_{33} = -0.0144 \\ \varepsilon_{22} = 0.01979 \end{cases} \qquad Ni \quad \begin{cases} \varepsilon_{11} = \varepsilon_{33} = 0.01223 \\ \varepsilon_{22} = -0.01487 \end{cases}$$

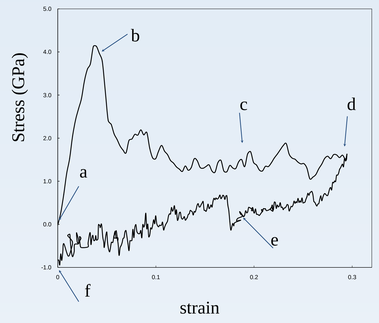
✓EAM potential: CuNiH.eam
✓Temperature: 300K
✓Uniaxial tensile loading
✓Boundary conditions:
is fixed at the bottom

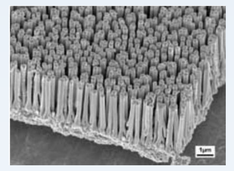


Results

a <110>/{111}4.17nm x4.17nm composite nanowire during loading and unloading at the temperature of 300K

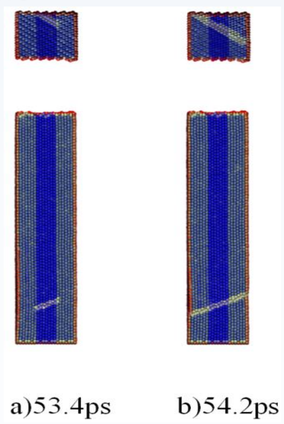




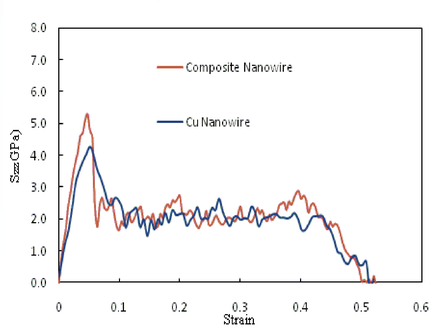


A forest of copper rods about 100 nanometers

Initiation of the first twin boundary from the free surface and at the interface of the layers



the presence of the coherent interface results in an increase in the yield stress



Conclusion

by utilizing molecular dynamics simulations, we have shown that:

➢Unlike the single crystalline nanowires in which the twins initiate from the sharp edges of free surfaces, in composite nanowires the first twin boundary initiates at the interface and then propagates to the Ni layer and afterwards expands to the neighboring Cu layers.

➢Because of the coupled effects of geometry and coherent interface, the critical size is 6.5 times greater than that for single crystalline Cu nanowires.

➢composite nanowires offer stiffness enhancement compared to the corresponding monolithic Cu nanowires.

References

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