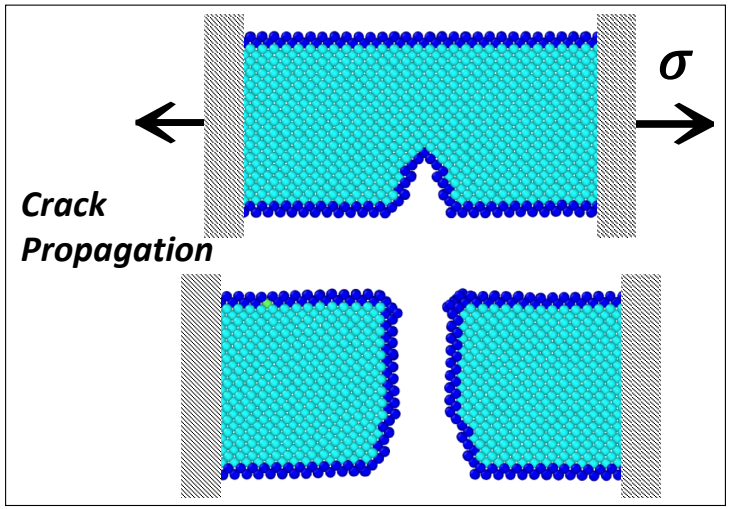
Nanomaterial Mechanics Explorer

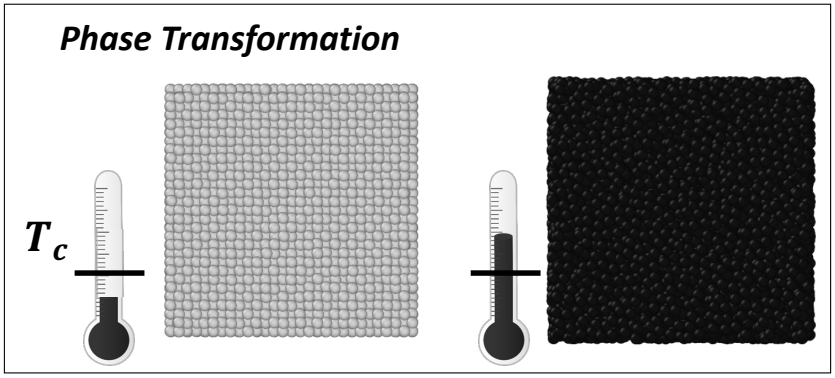
nanohub.org/tools/nanomatmech

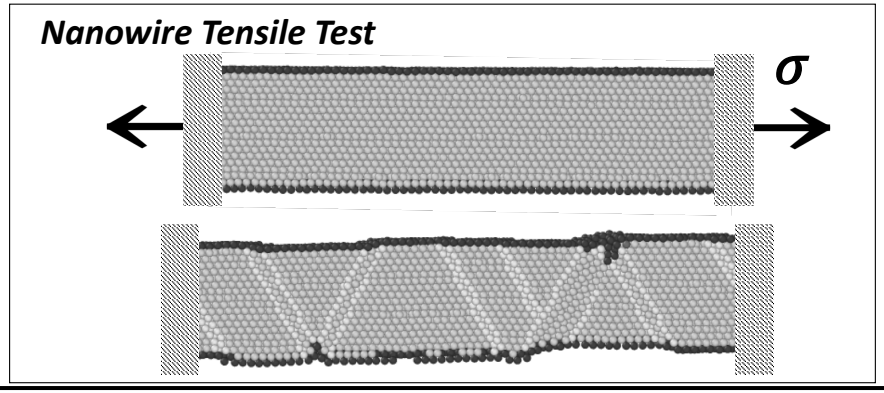
Default Run Simulation Details

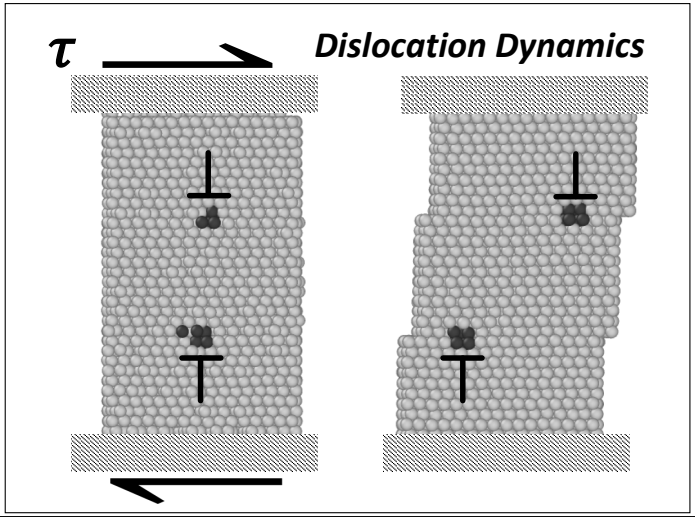
Ale Strachan (strachan@purdue.edu)
Michael Sakano, Shuhui Tang, Alexis Belessiotis, Mitch Wood,
Sam Reeve, Kiettipong Banlusan

School of Materials Engineering & Birck Nanotechnology Center
Purdue University
West Lafayette, Indiana USA









Crack Propagation Default Settings (1/4)

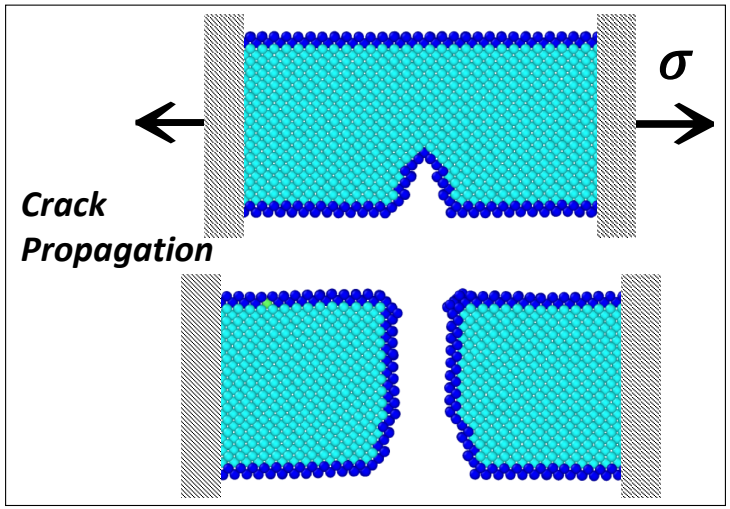
Material: Nickel (FCC) **Dimensions:** 10.6nm x 5.1nm x 1.8nm

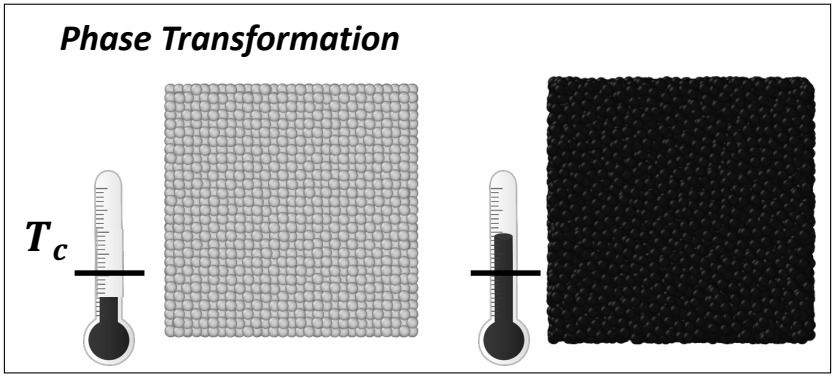
Flaw Shape: Triangle **Flaw Size:** 0.5nm length x 0.4nm width

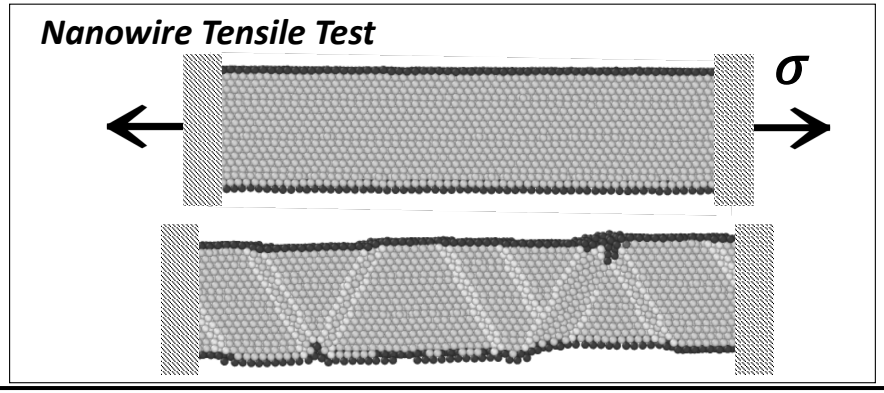
Orientation: x = [100] (Tensile Direction), y = [010], z = [001]

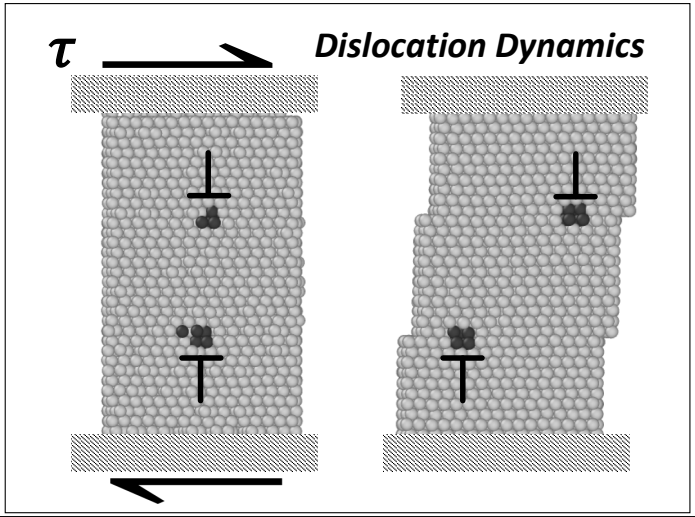
Temperature: 200K **Initial Stress:** 0.0 GPa

Total Simulation Time: 150ps **Strain Rate:** $1 \cdot 10^{-3}$ ps^{-1}









Crack Propagation Default Settings (2/4)

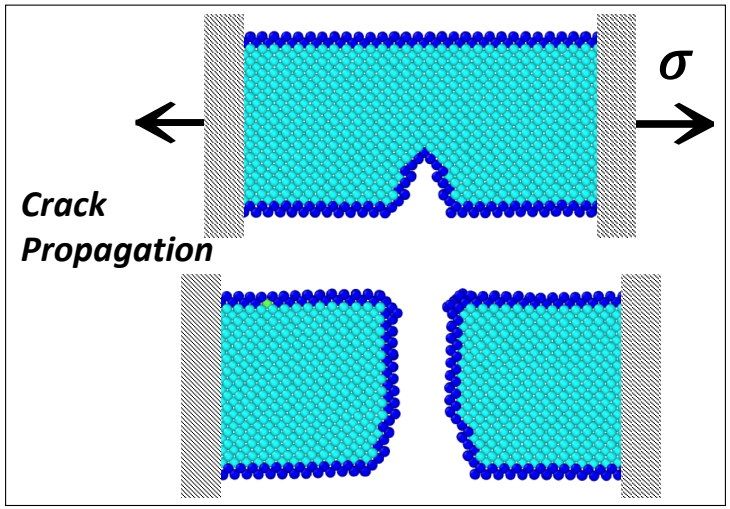
Material: Nickel (FCC) **Dimensions:** 10.6nm x 5.1nm x 1.8nm

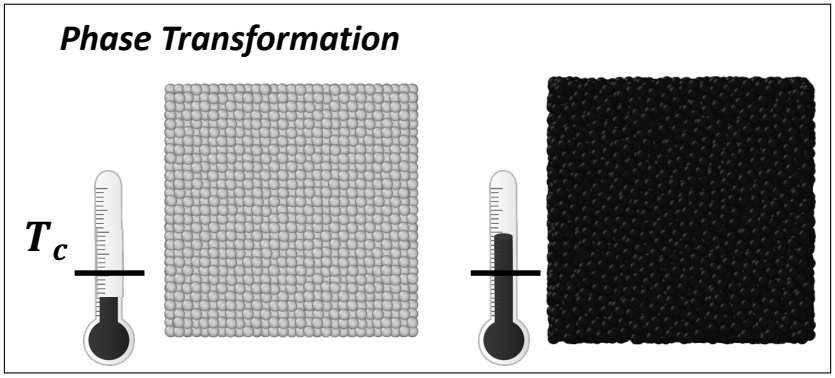
Flaw Shape: Triangle **Flaw Size:** 0.5nm length x 0.4nm width

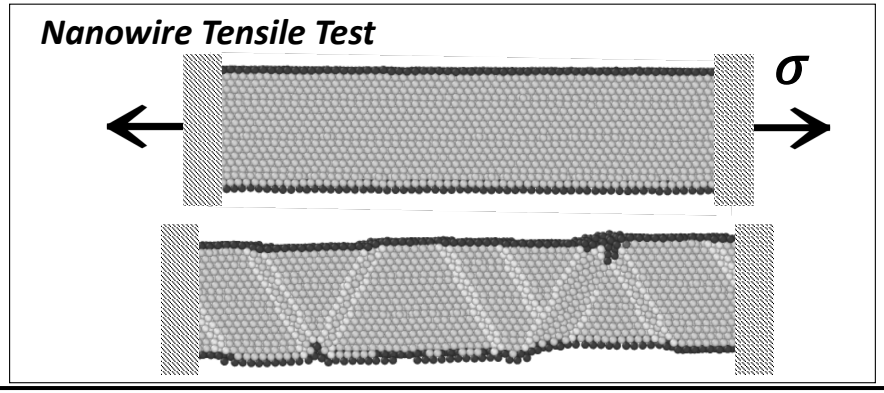
Orientation: x = [100] (Tensile Direction), y = [010], z = [001]

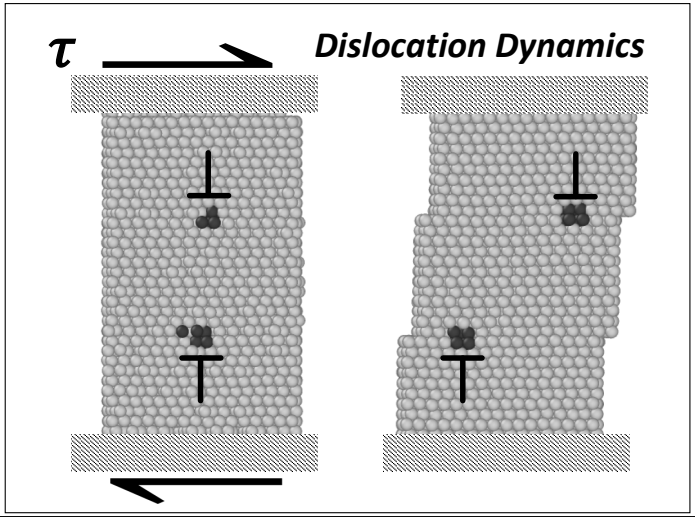
Temperature: 800K **Initial Stress:** 0.0 GPa

Total Simulation Time: 150ps **Strain Rate:** $1 \cdot 10^{-3}$ ps^{-1}









Crack Propagation Default Settings (3/4)

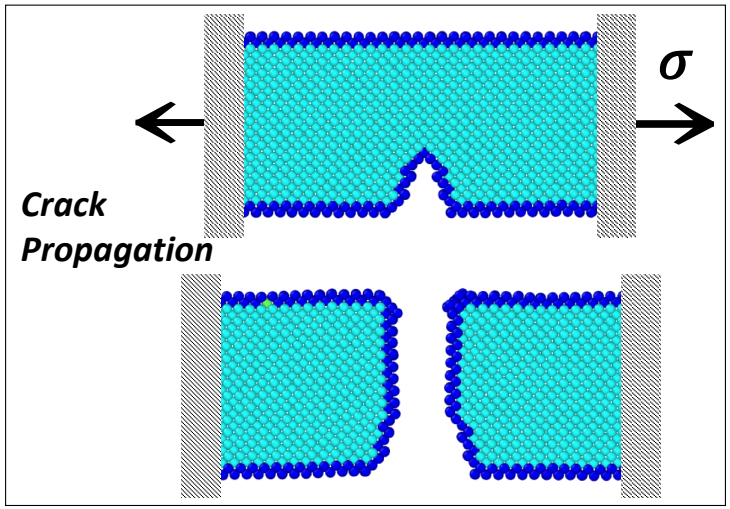
Material: ***Iron (BCC)*** ***Dimensions:*** *10.6nm x 5.1nm x 1.8nm*

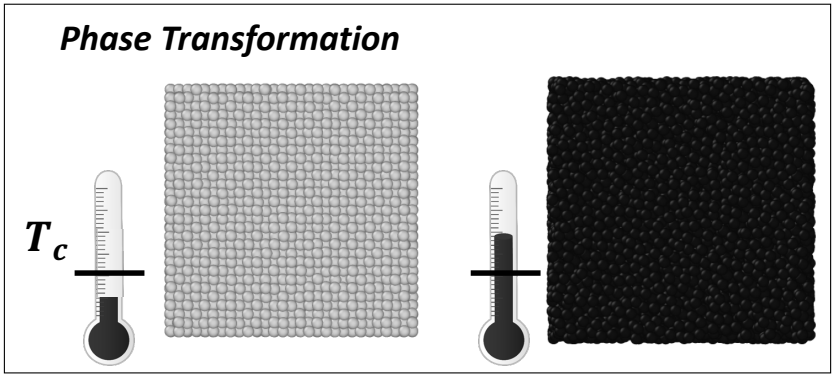
Flaw Shape: *Triangle* ***Flaw Size:*** *0.5nm length x 0.4nm width*

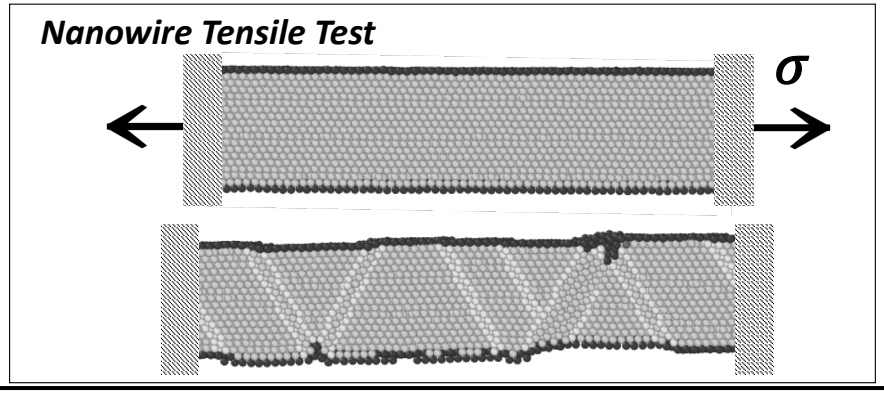
Orientation: *x = [100] (Tensile Direction), y = [010], z = [001]*

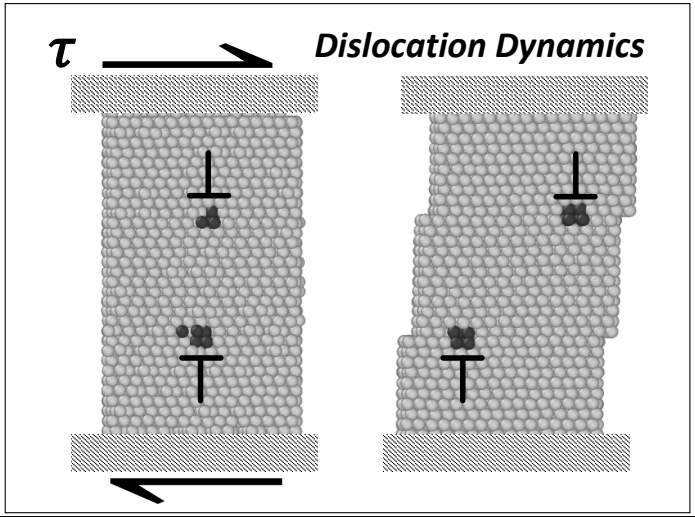
Temperature: ***200K*** ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *150ps* ***Strain Rate:*** $1 \cdot 10^{-3}$ ps^{-1}









Crack Propagation Default Settings (3/4)

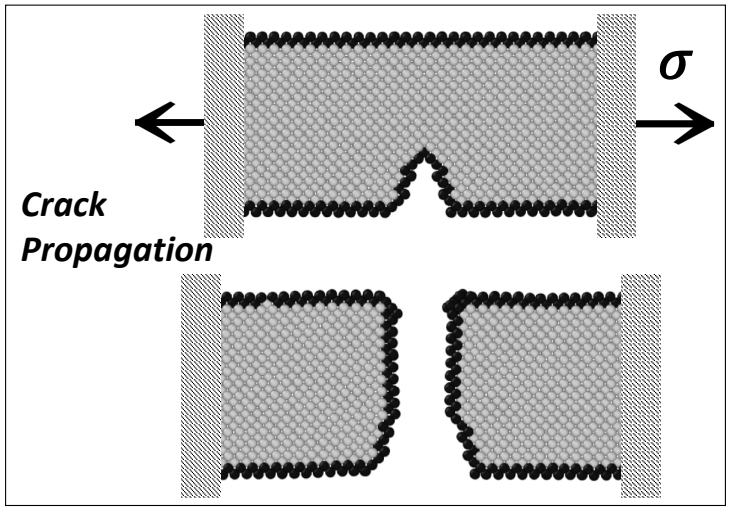
Material: ***Iron (BCC)*** ***Dimensions:*** *10.6nm x 5.1nm x 1.8nm*

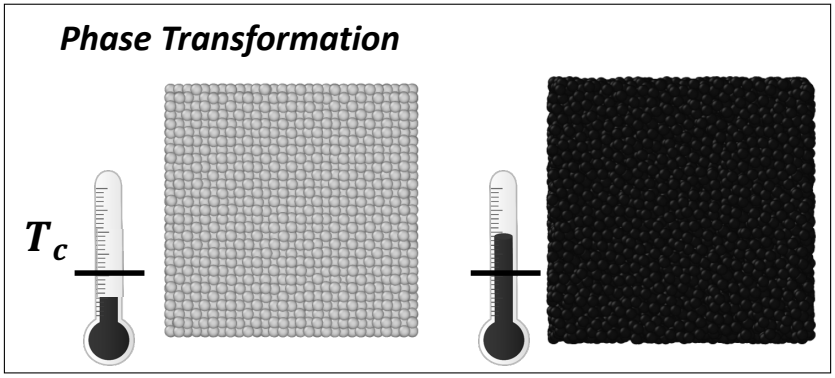
Flaw Shape: *Triangle* ***Flaw Size:*** *0.5nm length x 0.4nm width*

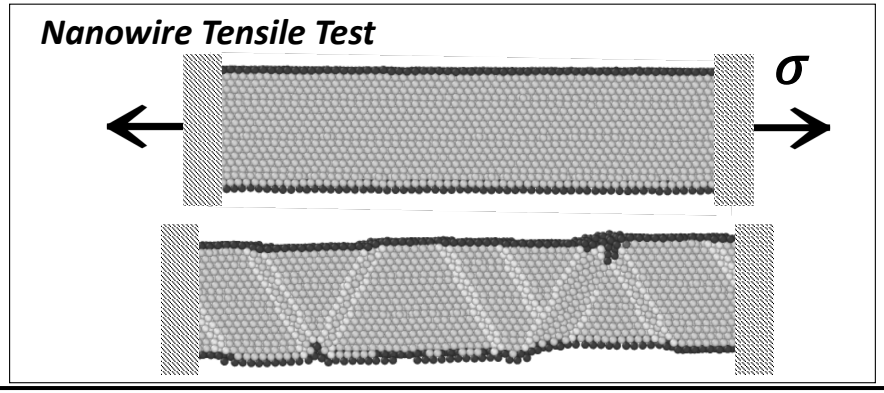
Orientation: *x = [100] (Tensile Direction), y = [010], z = [001]*

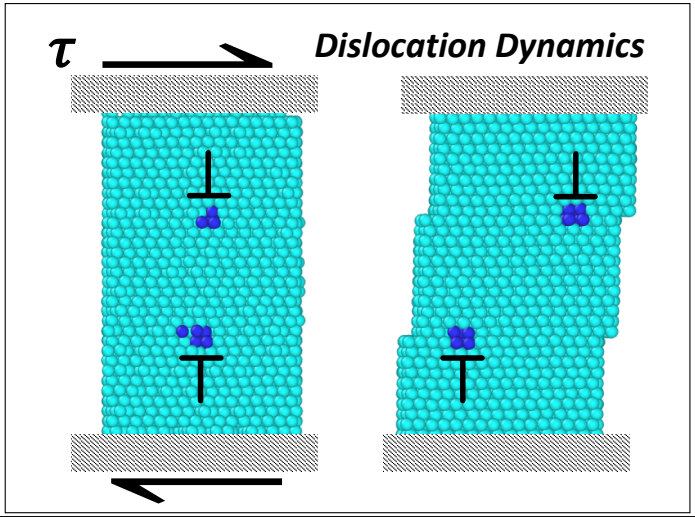
Temperature: ***800K*** ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *150ps* ***Strain Rate:*** $1 \cdot 10^{-3}$ ps^{-1}









Dislocation Dynamics Default Settings (1/5)

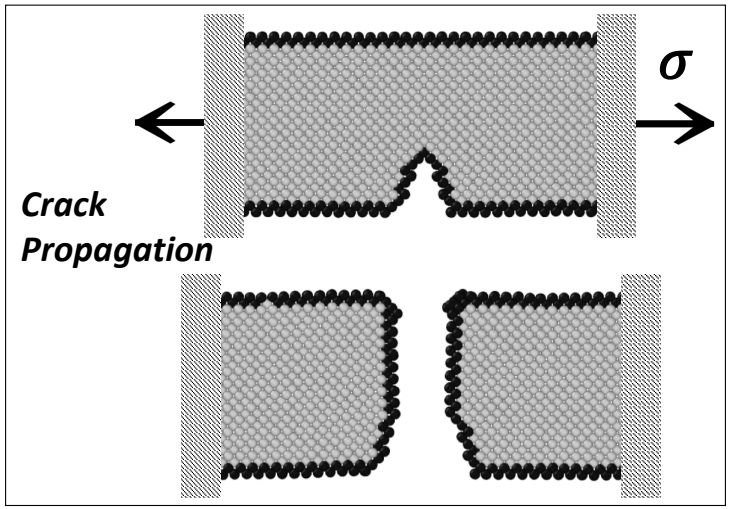
Material: ***Copper (FCC)*** ***Dimensions:*** *4.0nm x 7.5nm x 3.5nm*

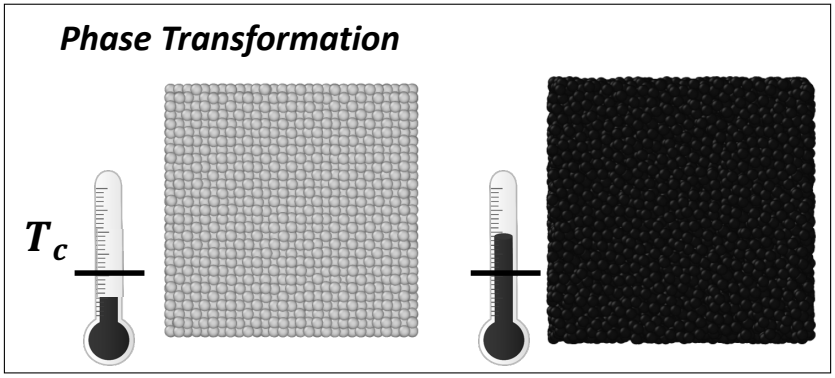
Dislocation Type: ***Edge*** ***Shear Stress:*** *xy*

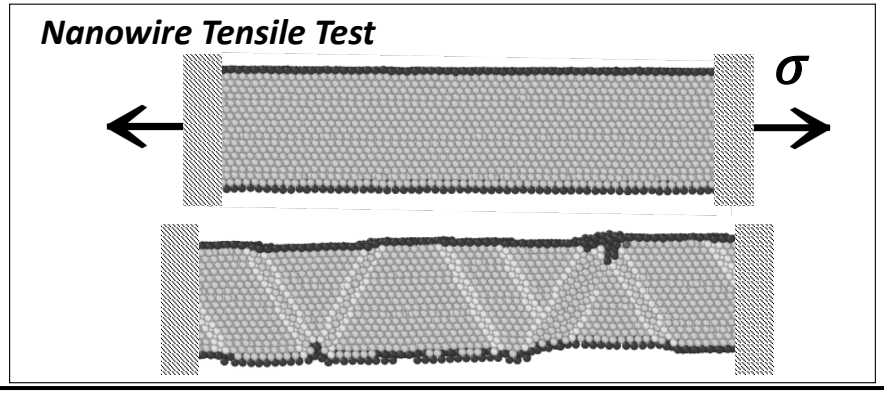
Orientation: *x = [-110], y = [111], z = [11-2]*

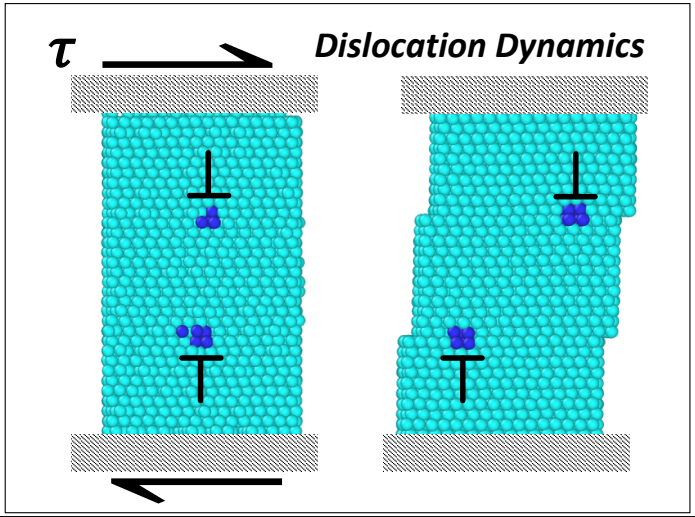
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *100ps* ***Strain Rate:*** $6 \cdot 10^{-2}$ ps^{-1}









Dislocation Dynamics Default Settings (2/5)

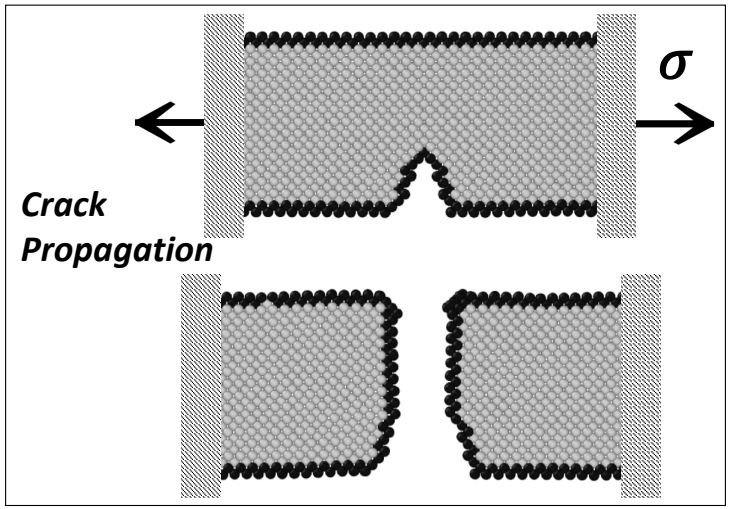
Material: Copper (FCC) **Dimensions:** 10.0nm x 1.8nm x 9.8nm

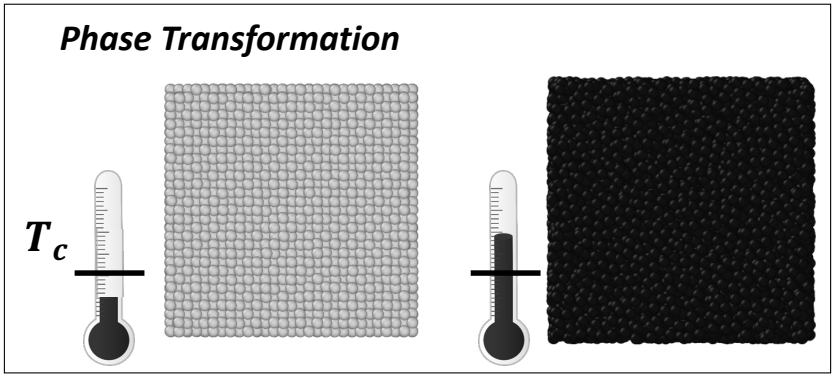
Dislocation Type: Screw (dissociated) **Shear Stress:** yz

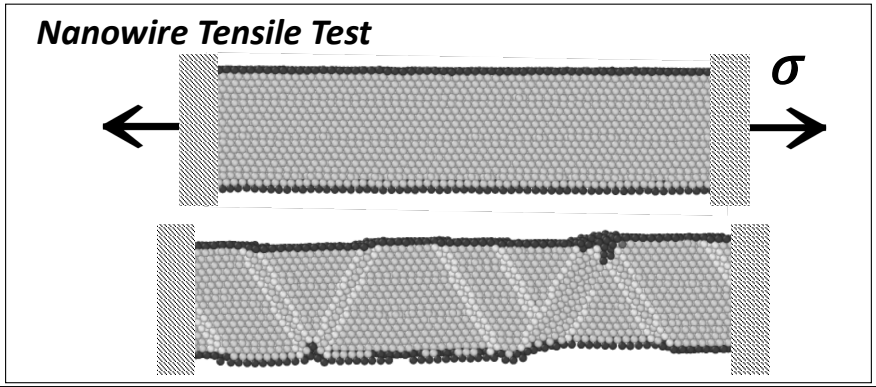
Orientation: x = [111], y = [1-10], z = [11-2]

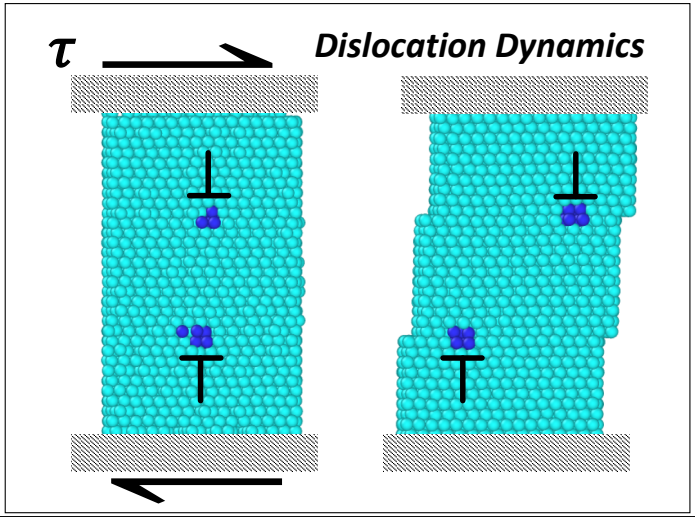
Temperature: 300K **Initial Stress:** 0.0 GPa

Total Simulation Time: 100ps **Strain Rate:** $3 \cdot 10^{-2}$ ps^{-1}









Dislocation Dynamics Default Settings (3/5)

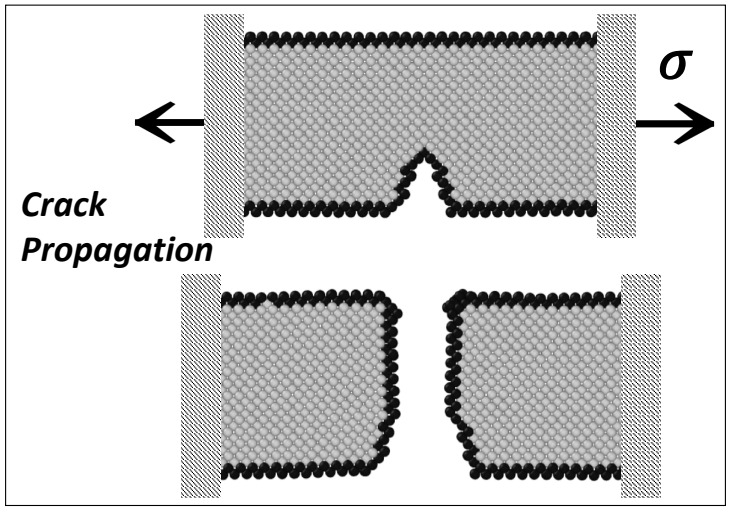
Material: ***Copper (FCC)*** ***Dimensions:*** *10.0nm x 2.0nm x 9.8nm*

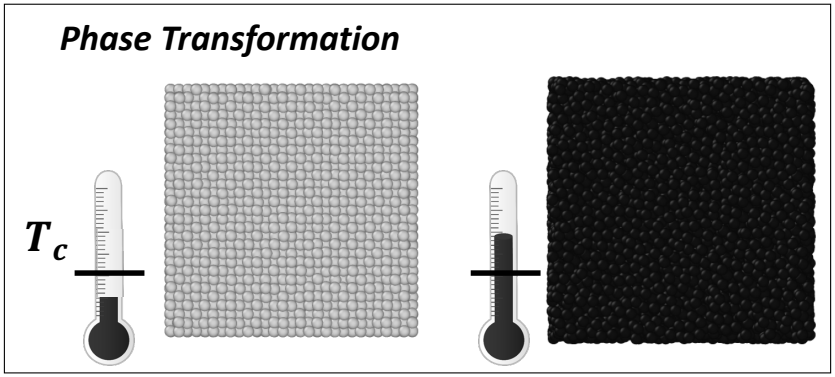
Dislocation Type: ***Screw*** ***Shear Stress:*** *yz*

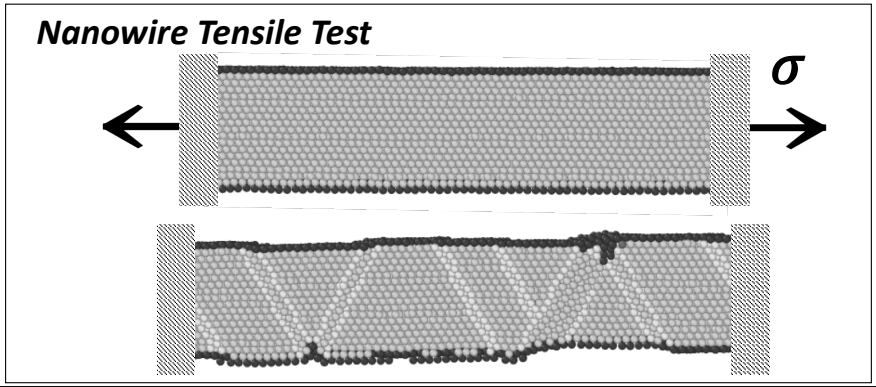
Orientation: *x = [111], y = [1-10], z = [11-2]*

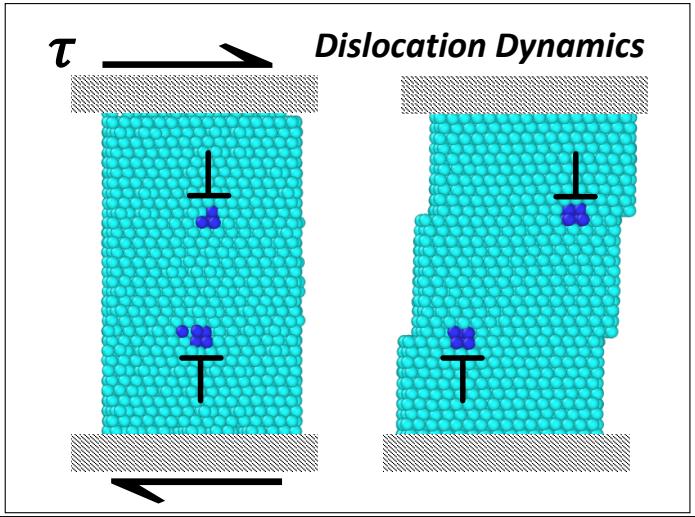
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *100ps* ***Strain Rate:*** $2 \cdot 10^{-2}$ ps^{-1}









Dislocation Dynamics Default Settings (4/5)

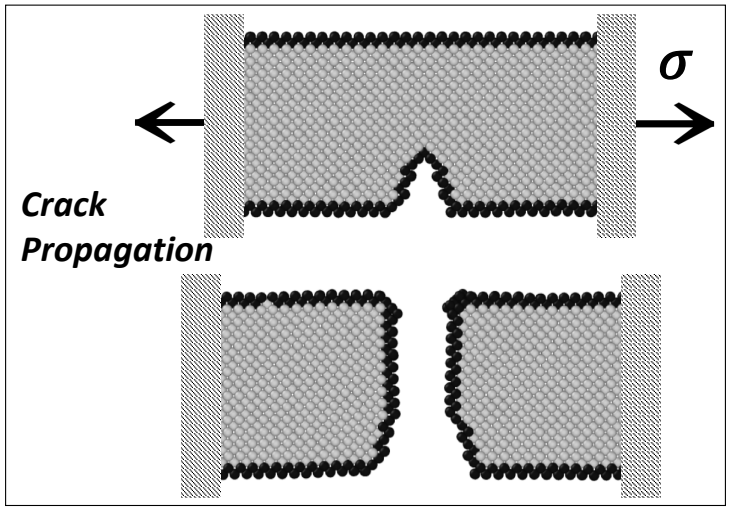
Material: ***Iron (BCC)*** ***Dimensions:*** *8.5nm x 2.0nm x 8.4nm*

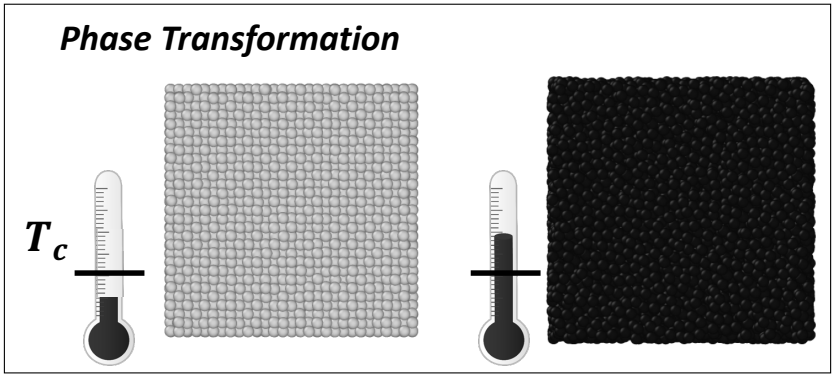
Dislocation Type: ***Edge*** ***Shear Stress:*** *xy*

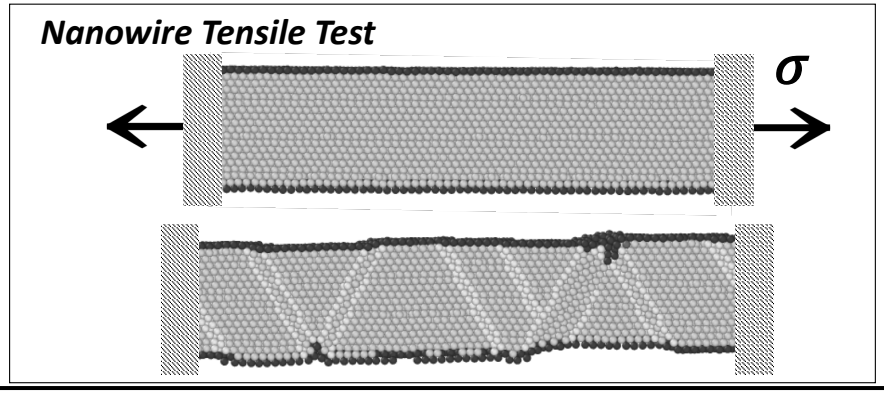
Orientation: *x = [111], y = [1-10], z = [11-2]*

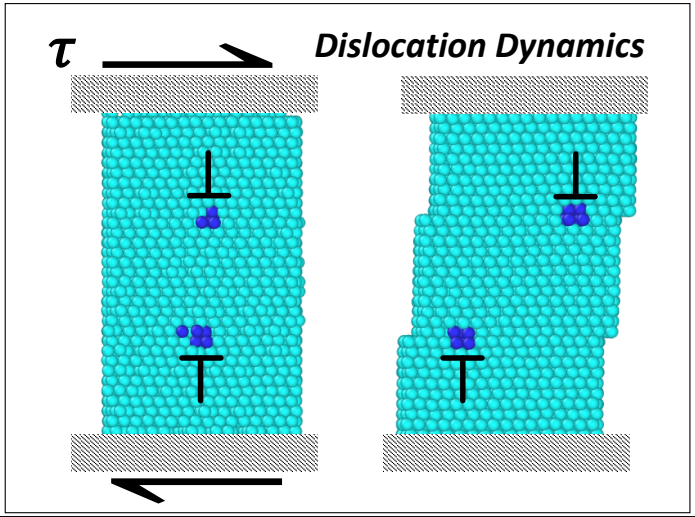
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *100ps* ***Strain Rate:*** $8 \cdot 10^{-2}$ ps^{-1}









Dislocation Dynamics Default Settings (5/5)

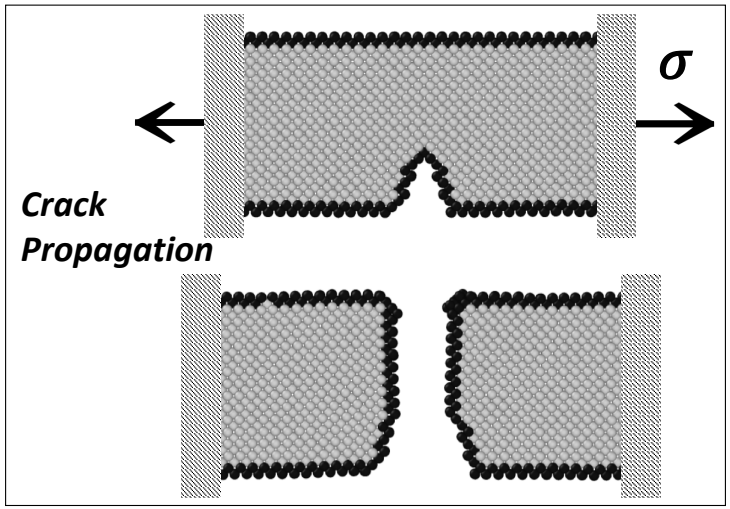
Material: ***Iron (BCC)*** ***Dimensions:*** *4.0nm x 6.5nm x 2.8nm*

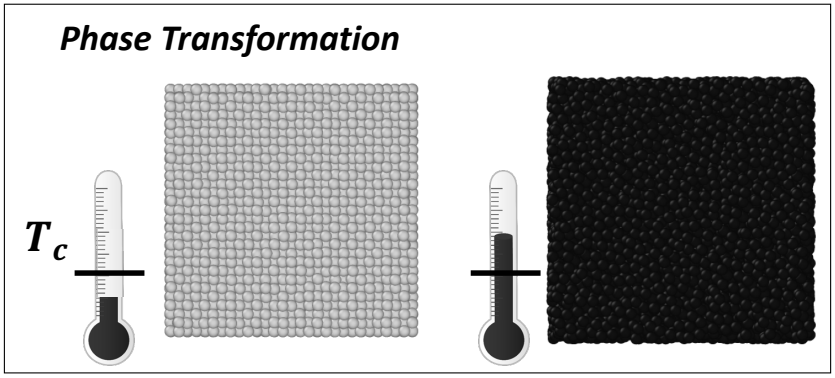
Dislocation Type: ***Screw*** ***Shear Stress:*** *yz*

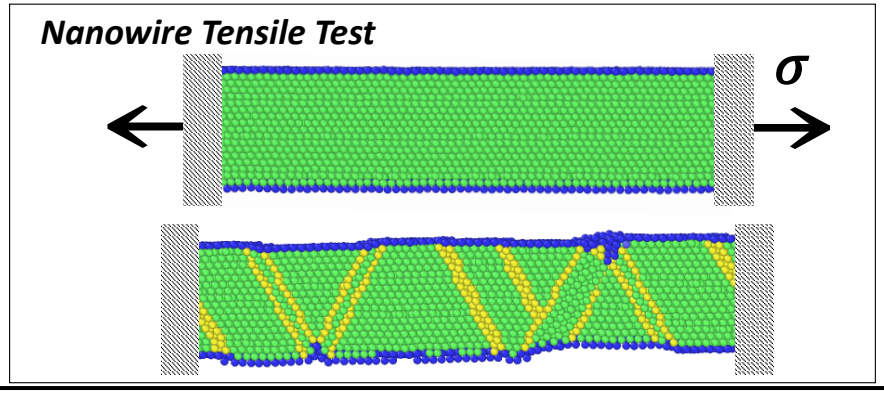
Orientation: *x = [-110], y = [111], z = [11-2]*

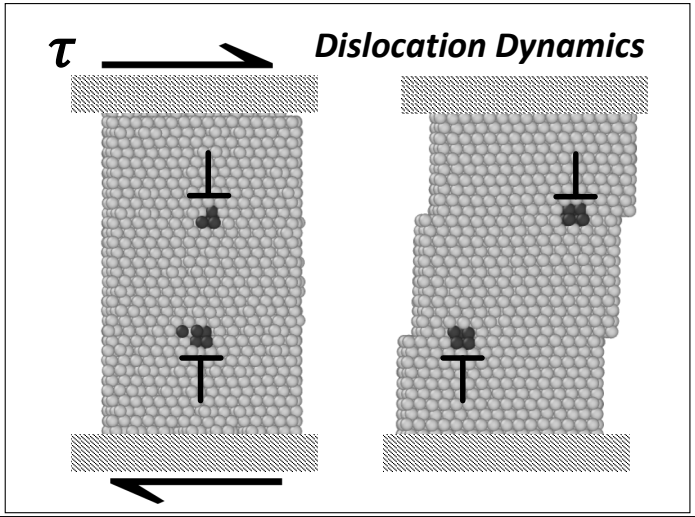
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *100ps* ***Strain Rate:*** $3 \cdot 10^{-2}$ ps^{-1}









Nanowire Tensile Test Default Settings (1/6)

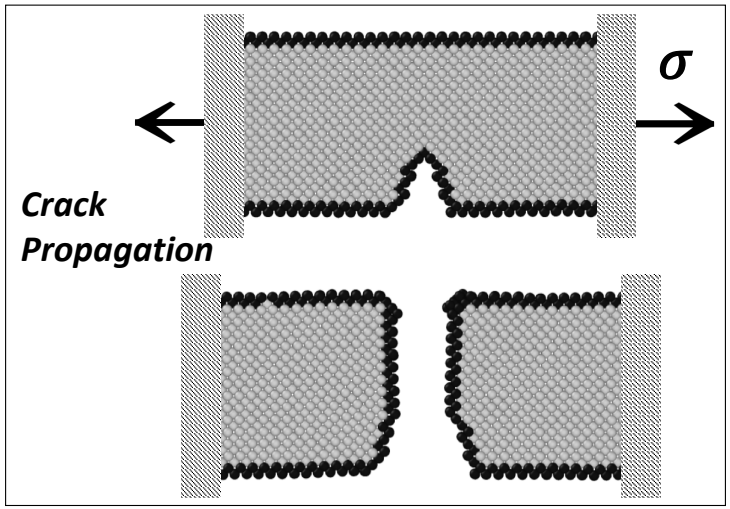
Material: ***Nickel (FCC)***

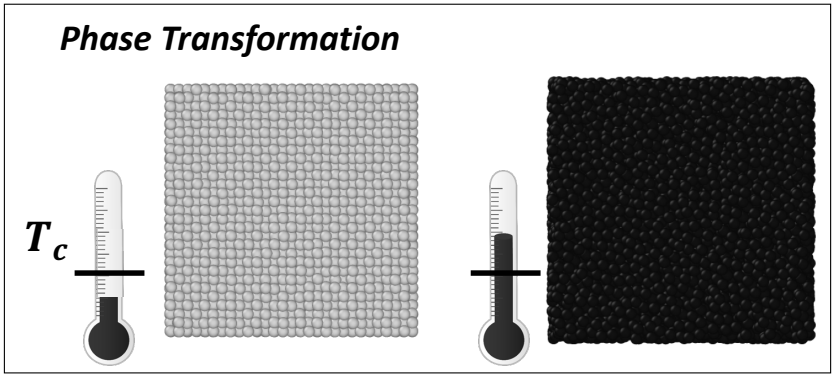
Dimensions: *15.5nm long, 3.7nm diameter wire*

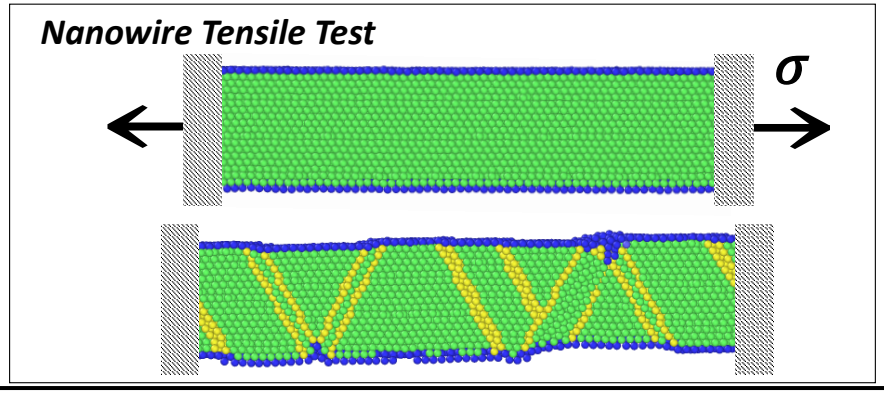
Orientation: ***x = [100] (Tensile Direction)****, y = [010], z = [001]*

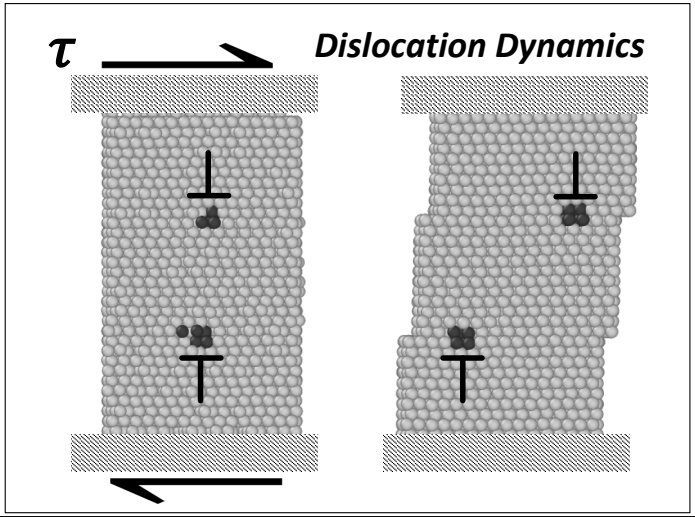
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-3}$ ps^{-1}









Nanowire Tensile Test Default Settings (2/6)

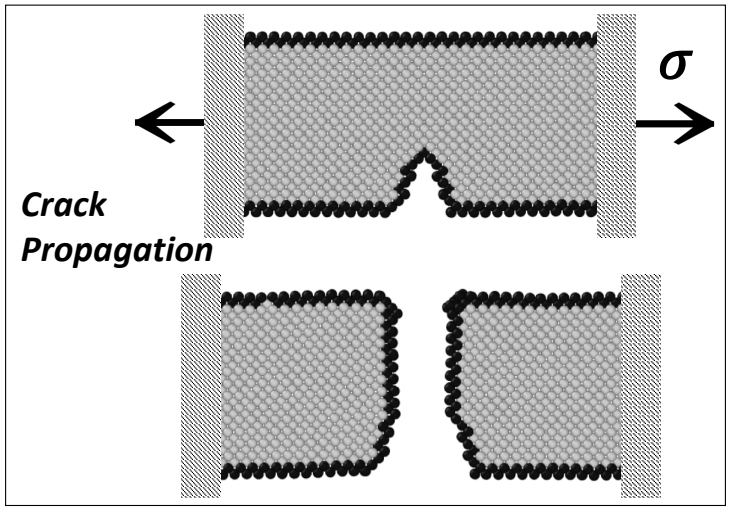
Material: ***Aluminum (FCC)***

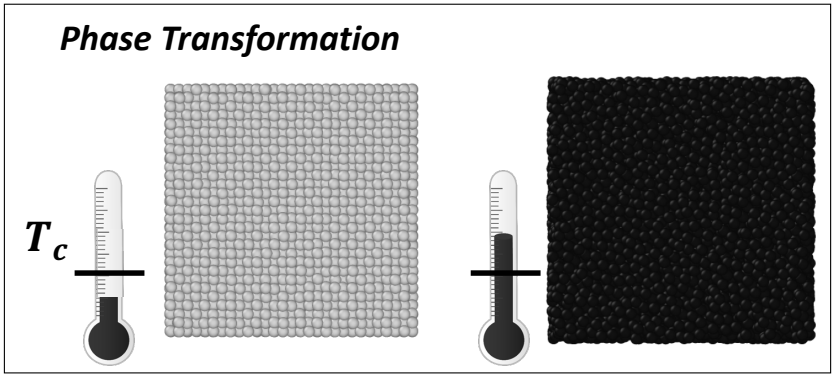
Dimensions: *15.5nm long, 3.7nm diameter wire*

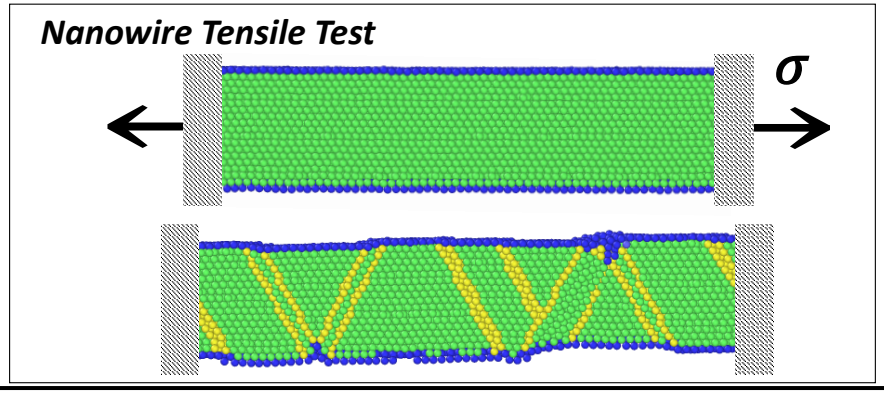
Orientation: ***x = [100] (Tensile Direction)****, y = [010], z = [001]*

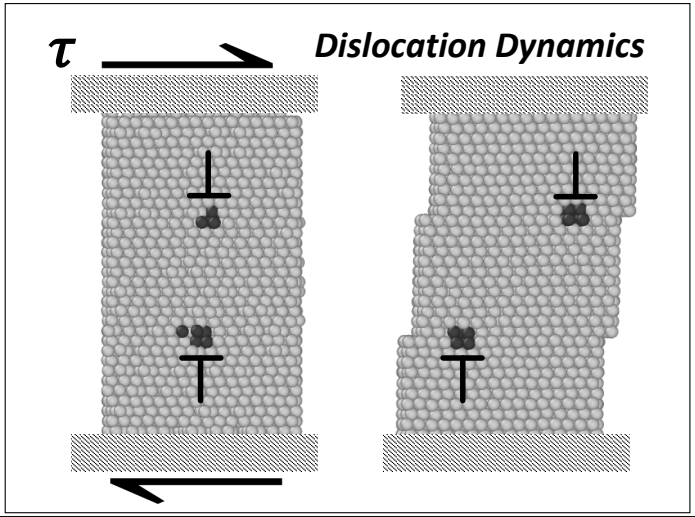
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-3}$ ps^{-1}









Nanowire Tensile Test Default Settings (2/6)

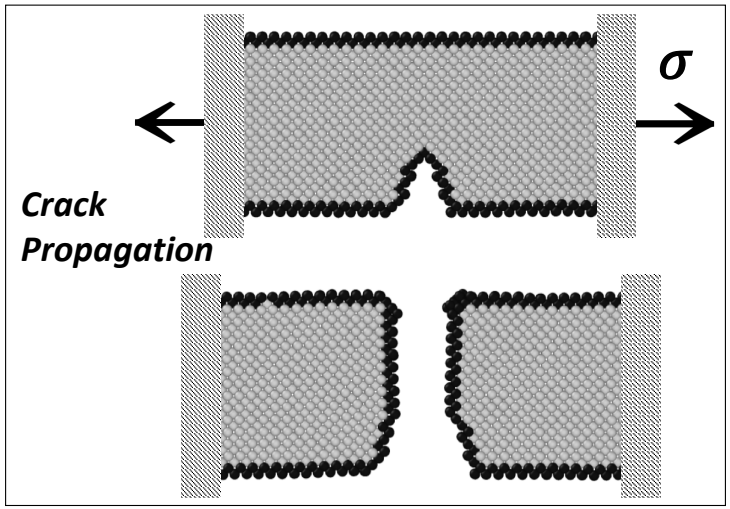
Material: ***Copper (FCC)***

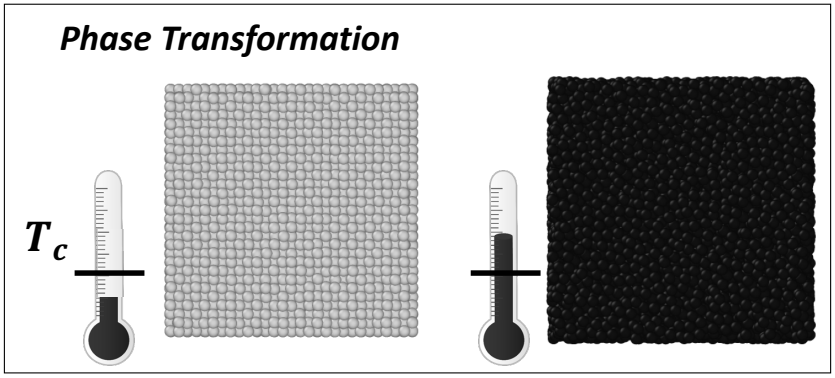
Dimensions: *15.5nm long, 3.7nm diameter wire*

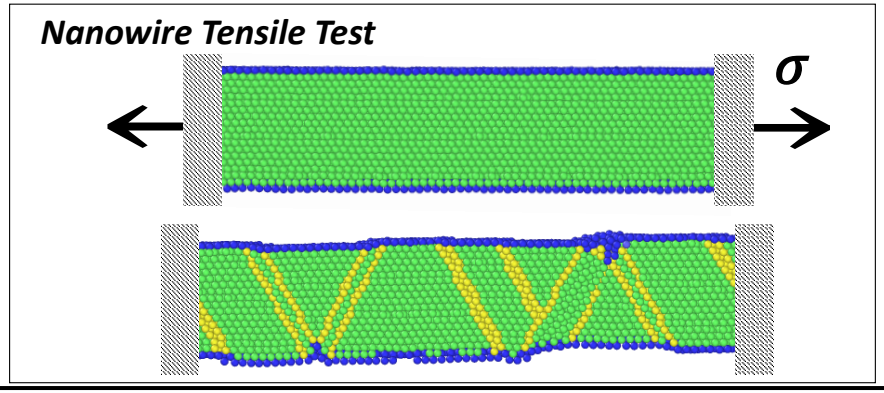
Orientation: ***x = [100] (Tensile Direction)****, y = [010], z = [001]*

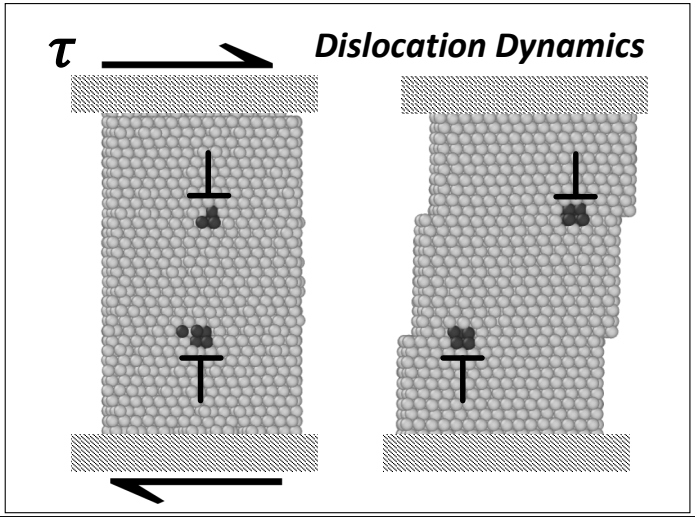
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-3}$ ps^{-1}









Nanowire Tensile Test Default Settings (2/6)

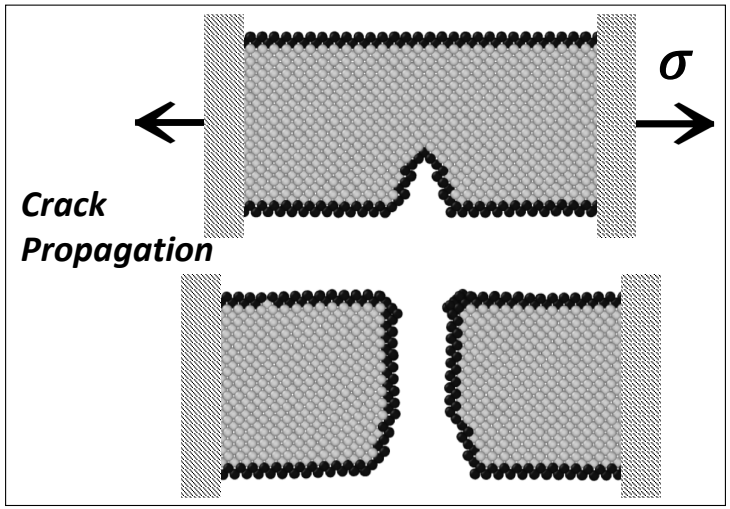
Material: ***Copper (FCC)***

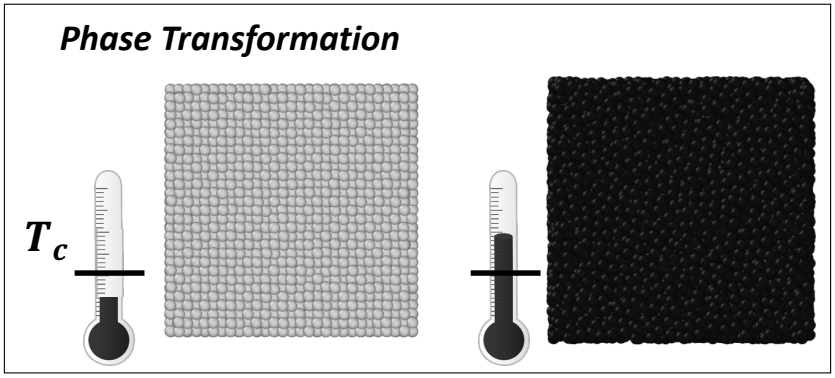
Dimensions: *15.5nm long, 3.7nm diameter wire*

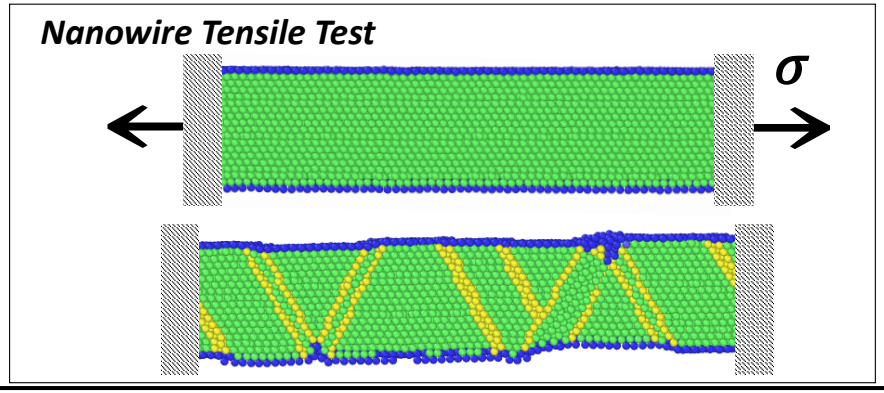
Orientation: ***x = [-110] (Tensile Direction)****, y = [111], z = [11-2]*

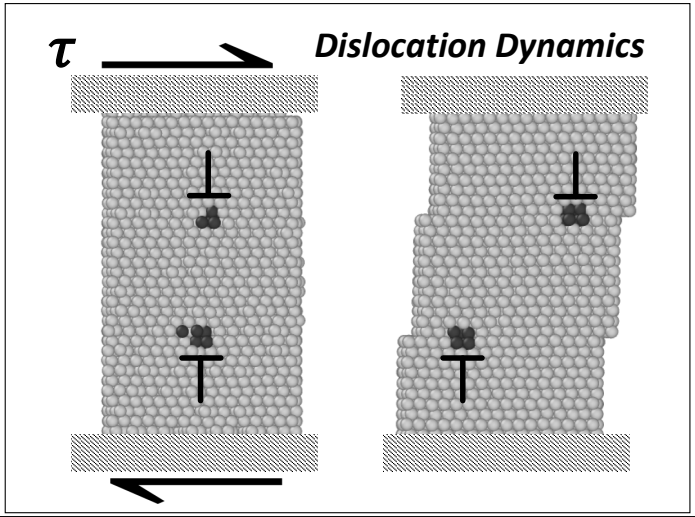
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-3}$ ps^{-1}









Nanowire Tensile Test Default Settings (2/6)

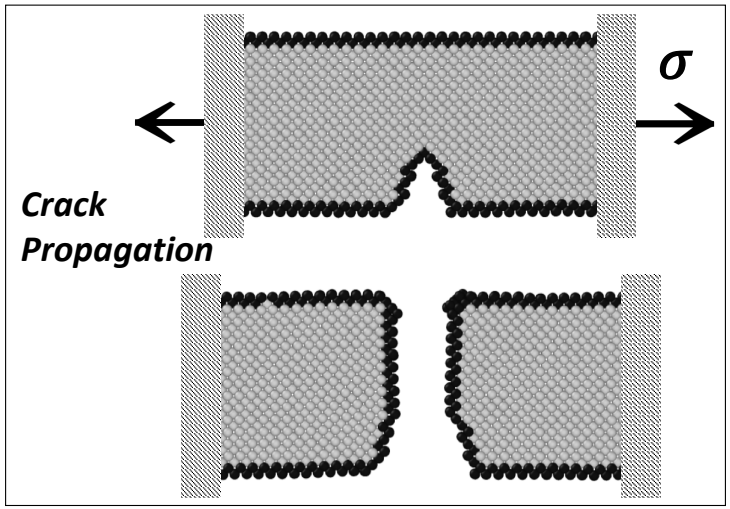
Material: ***Copper (FCC)***

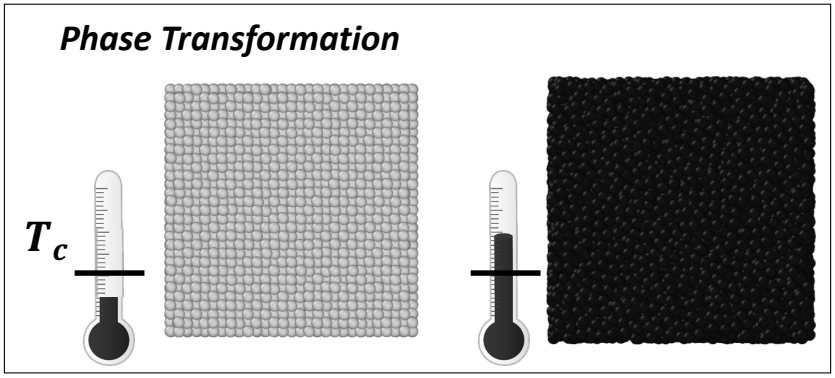
Dimensions: *15.5nm long, 3.7nm diameter wire*

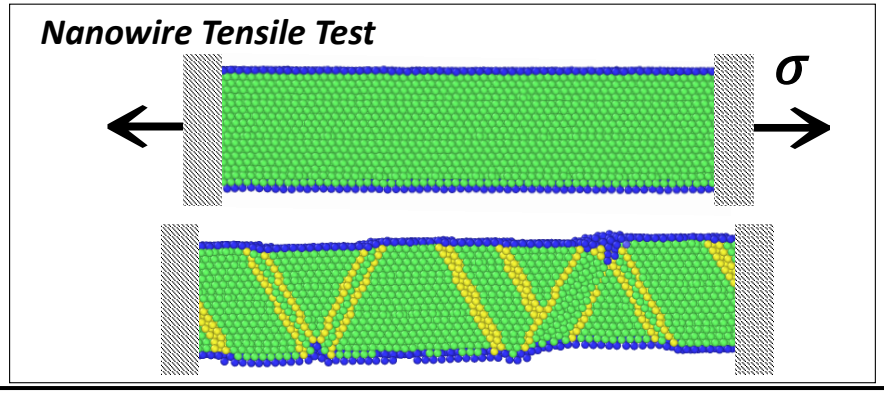
Orientation: ***x = [111] (Tensile Direction)****, y = [1-10], z = [11-2]*

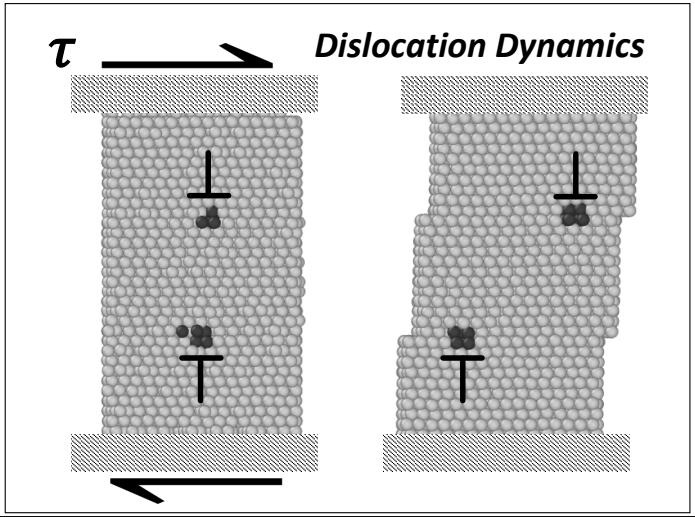
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-3}$ ps^{-1}









Nanowire Tensile Test Default Settings (2/6)

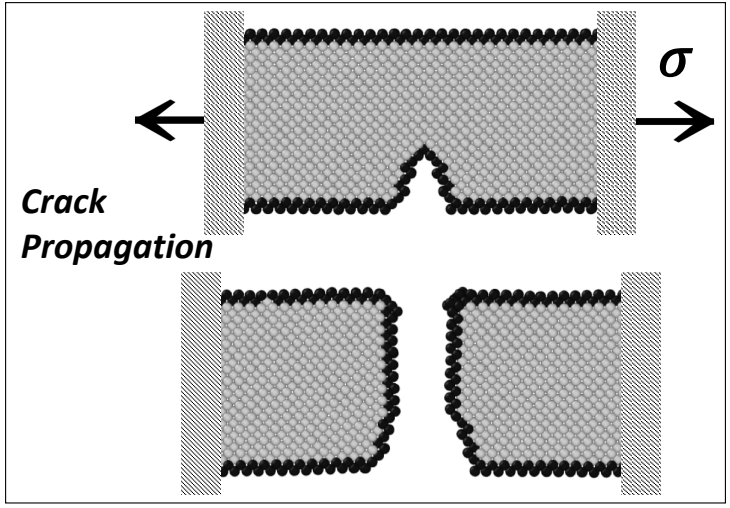
Material: ***Copper (FCC)***

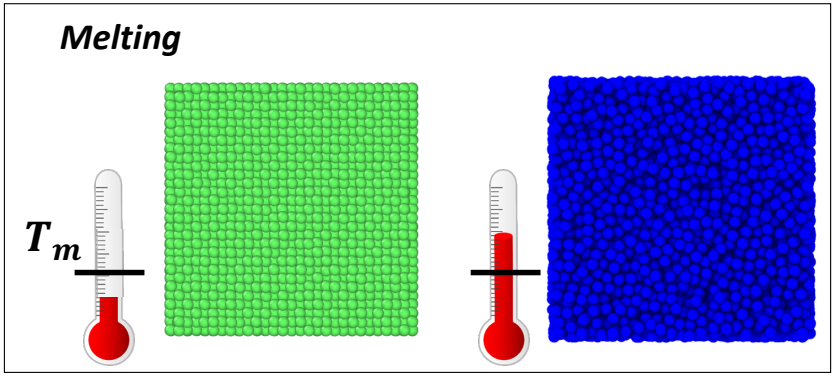
Dimensions: *15.5nm long, 3.7nm diameter wire*

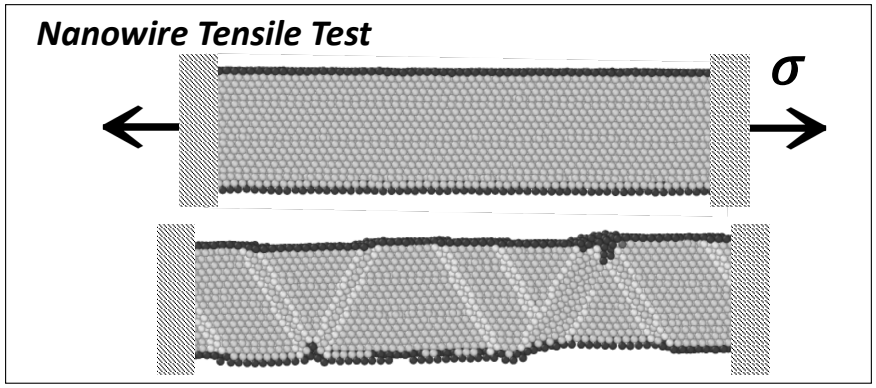
Orientation: ***x = [11-2] (Tensile Direction)****, y = [1-10], z = [111]*

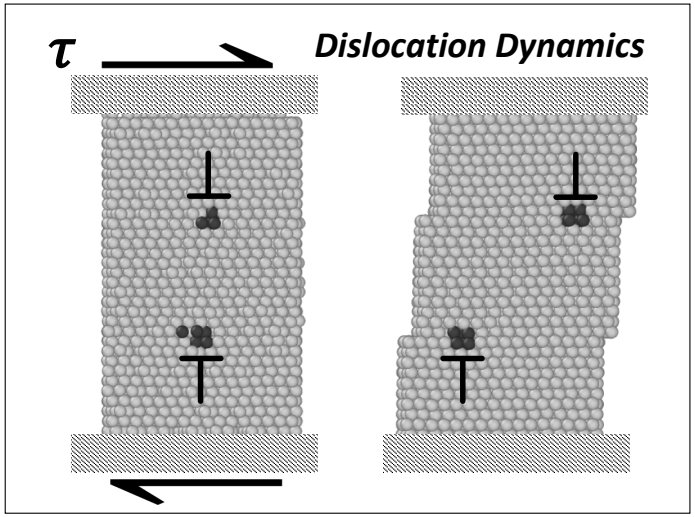
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-3}$ ps^{-1}









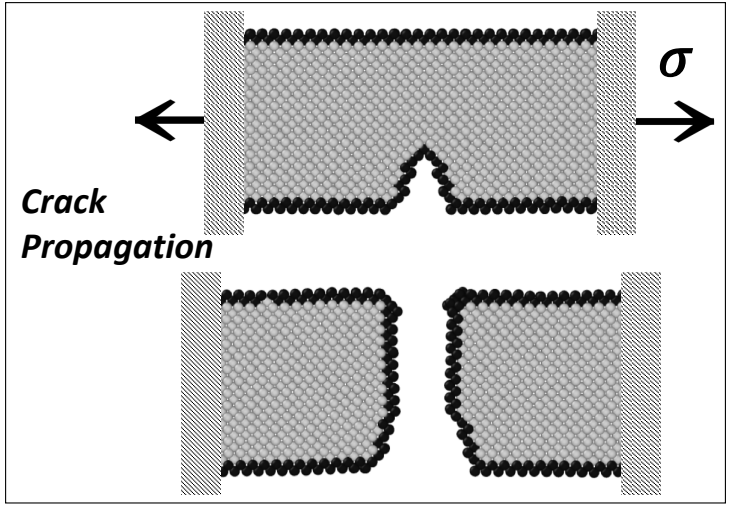
Melting Default Settings (1/2)

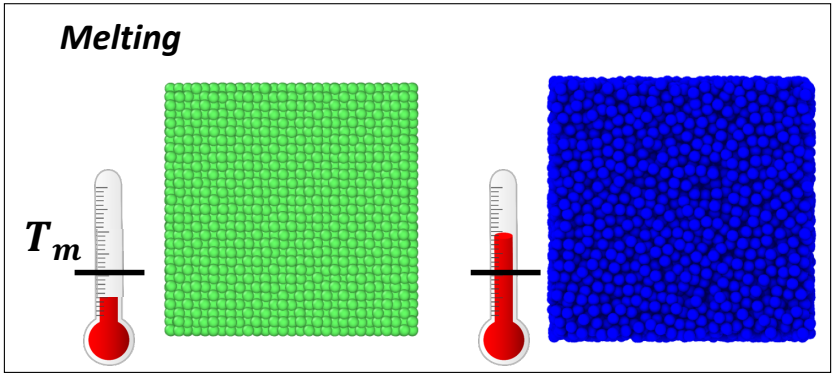
Material: *Nickel (FCC)* ***Dimensions:*** *4.9nm cube* ***(Bulk system)***

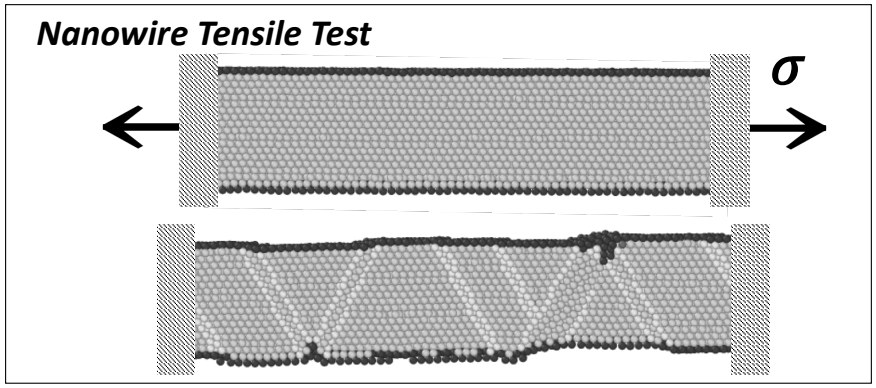
Orientation: *x = [100], y = [010], z = [001]*

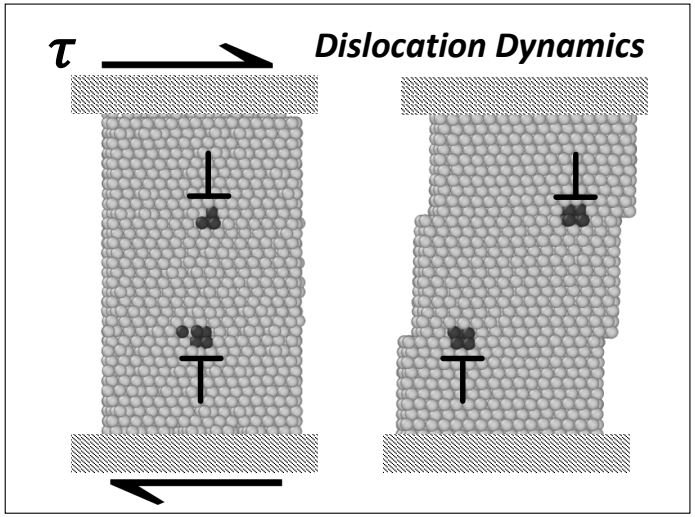
Temperature: *Heating from 300K to 2300K*

Total Simulation Time: *50ps* ***Initial Stress:*** *0.0 GPa*









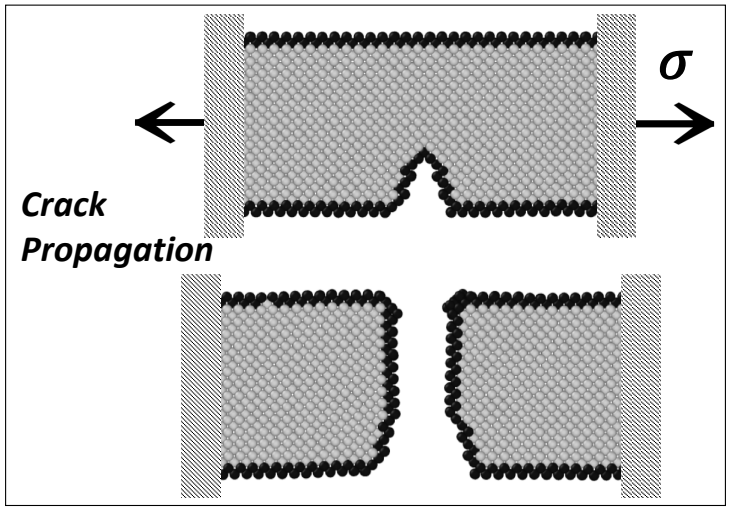
Melting Default Settings (2/2)

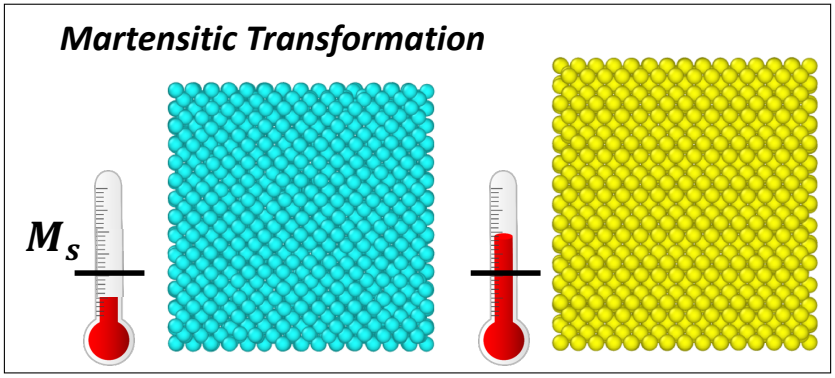
Material: *Nickel (FCC)* ***Dimensions:*** *4.8nm cube* ***(Nanoparticle)***

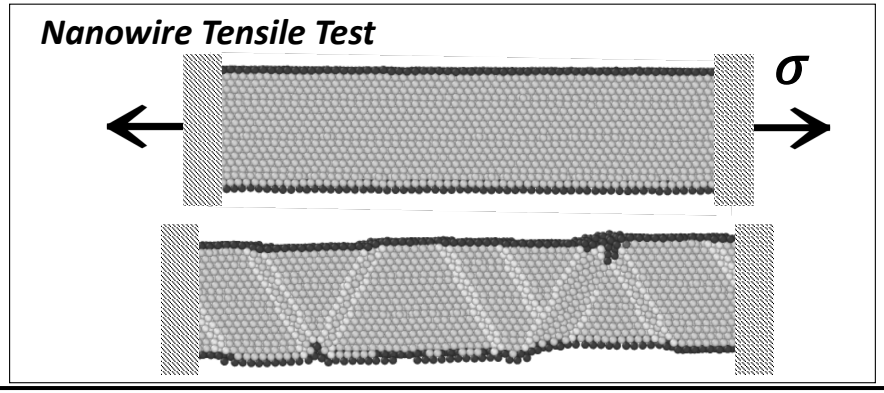
Orientation: *x = [100], y = [010], z = [001]*

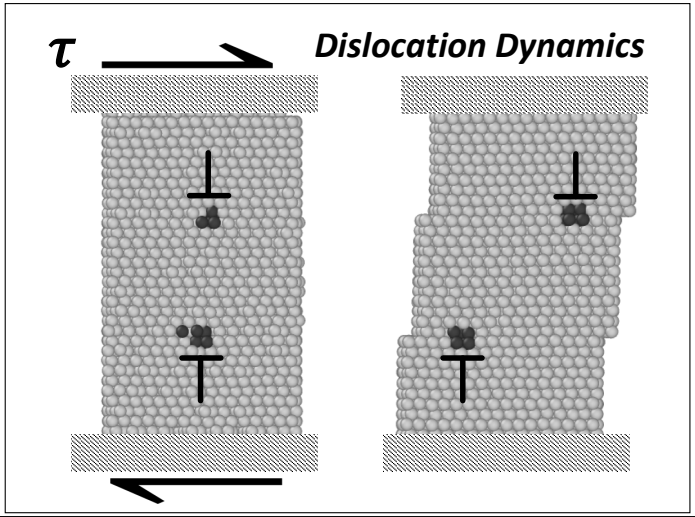
Temperature: *Heating from 300K to 2300K*

Total Simulation Time: *50ps* ***Initial Stress:*** *0.0 GPa*









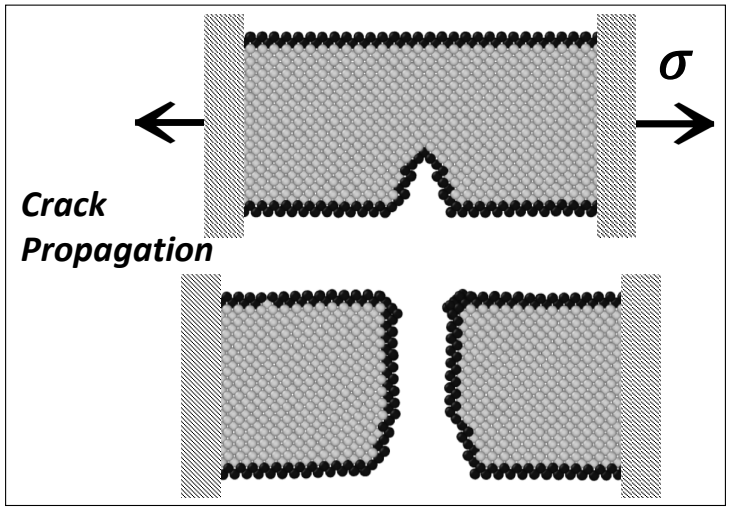
Martensitic Transformation Default Settings (1/4)

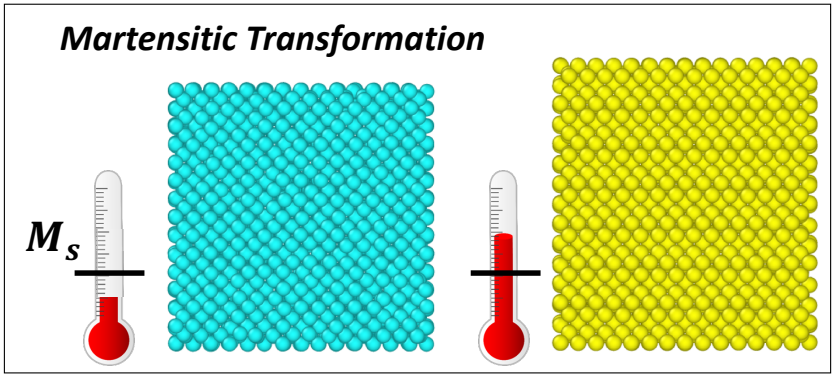
Material: $Ni_{0.63}Al_{0.37}$ ***random B2 alloy*** ***Dimensions:*** *4.1nm cube*

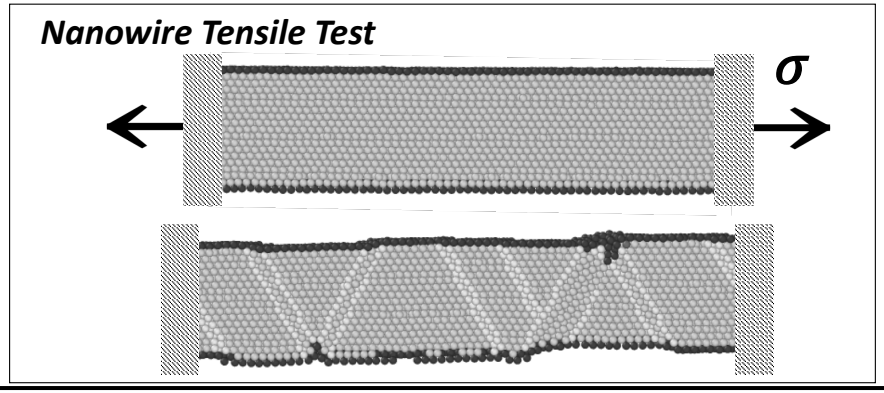
Orientation: *x = [100], y = [010], z = [001]*

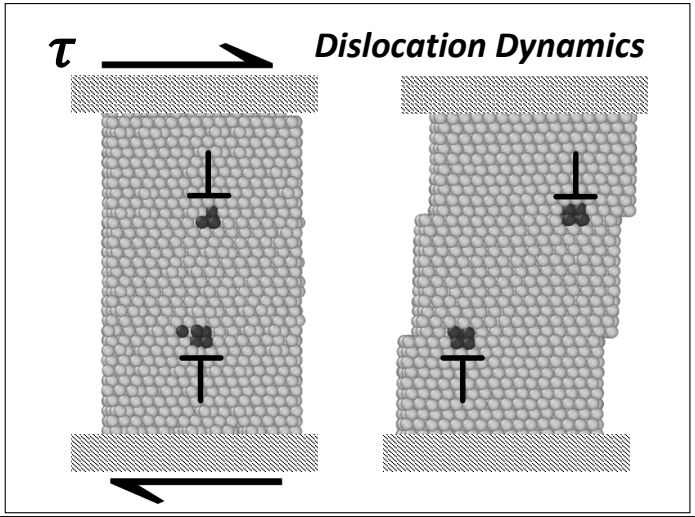
Temperature: *Cooling from 500K to 25K*

Total Simulation Time: *100ps* ***Initial Stress:*** *0.0 GPa*









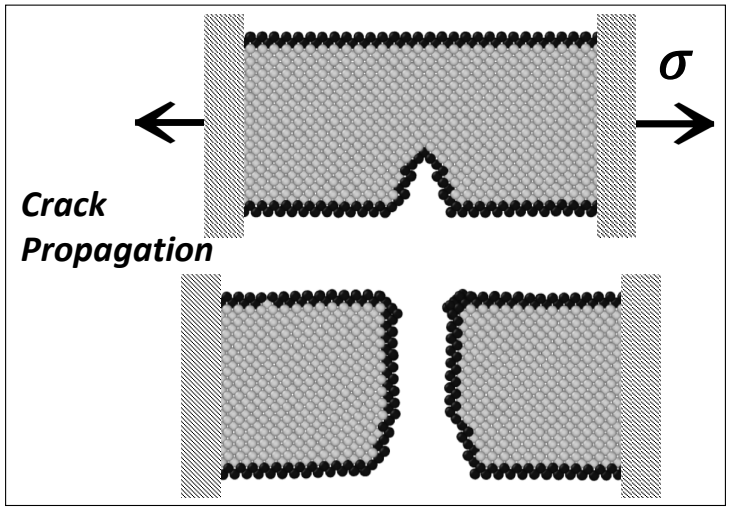
Martensitic Transformation Default Settings (2/4)

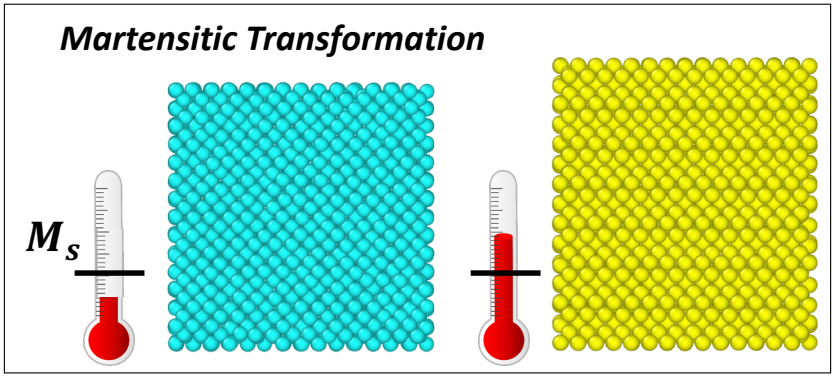
Material: ***$Ni_{0.50}Al_{0.50}$ B2 alloy*** ***Dimensions:*** *4.1nm cube*

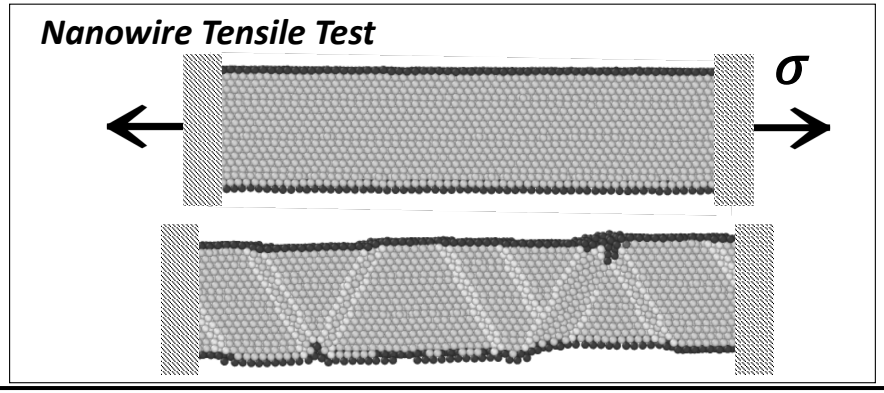
Orientation: *x = [100], y = [010], z = [001]*

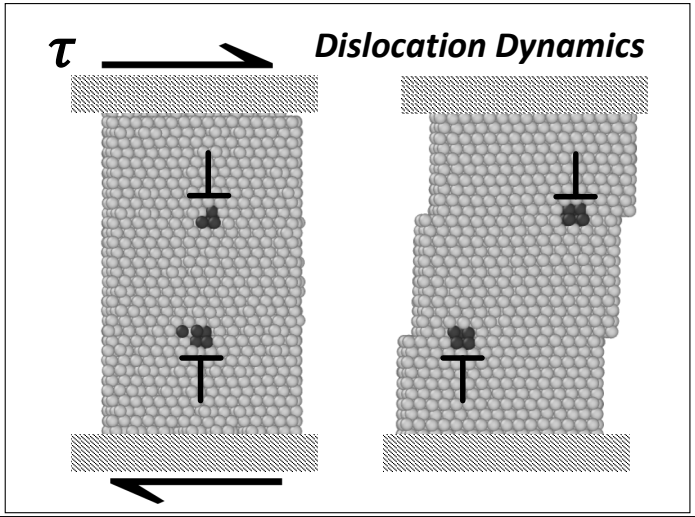
Temperature: *Cooling from 500K to 25K*

Total Simulation Time: *100ps* ***Initial Stress:*** *0.0 GPa*









Martensitic Transformation Default Settings (3/4)

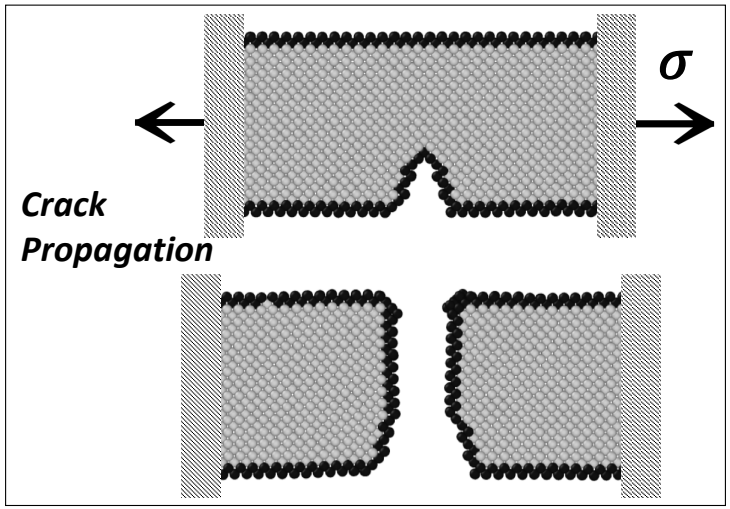
Material: ***$Ni_{0.63}Al_{0.37}$ random B2 alloy***

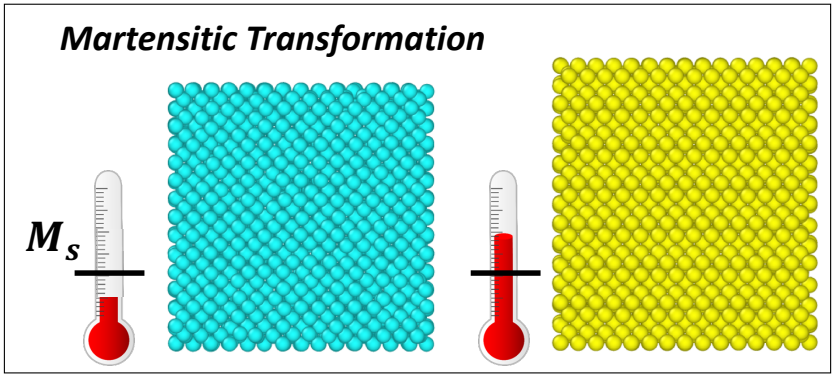
Dimensions: *55.0nm long, 7.4nm diameter wire*

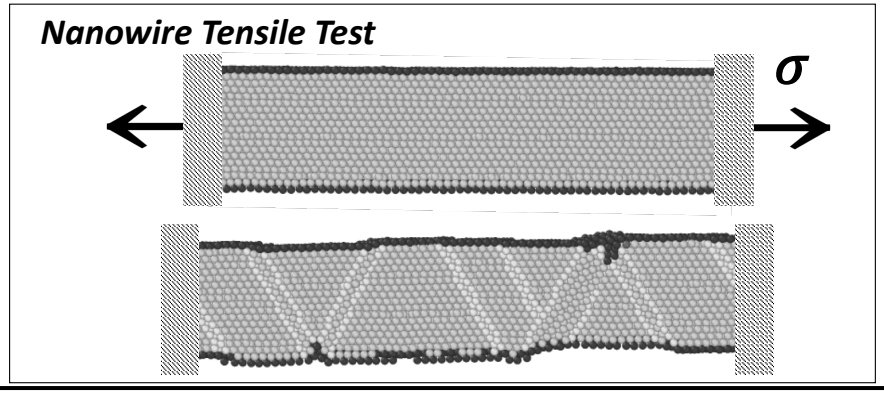
Orientation: *x = [100] (Tensile Direction), y = [010], z = [001]*

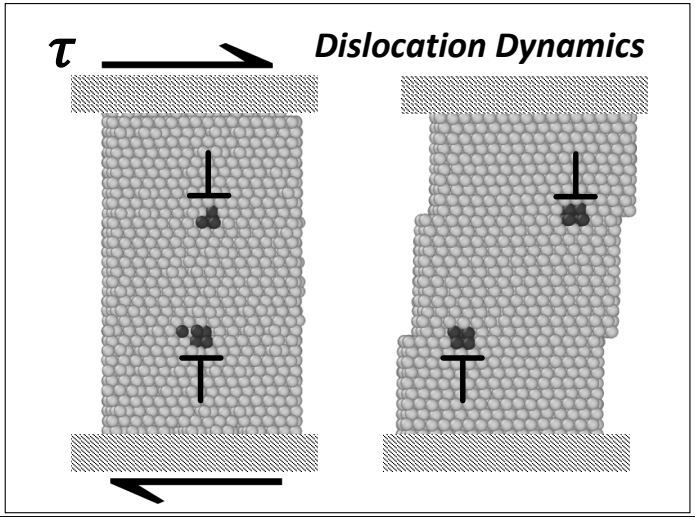
Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-4}$ ps^{-1}









Martensitic Transformation Default Settings (4/4)

Material: ***Metamaterial 70% $Ni_{0.63}Al_{0.37}$ random B2 / 30% $Ni_{0.50}Al_{0.50}$ B2***

Dimensions: *57.0nm long, 7.7nm diameter wire*

Orientation: *x = [100] (Tensile Direction), y = [010], z = [001]*

Temperature: *300K* ***Initial Stress:*** *0.0 GPa*

Total Simulation Time: *50ps* ***Strain Rate:*** $5 \cdot 10^{-4}$ ps^{-1}