JPPIPA 10(12) (2024)

Jurnal Penelitian Pendidikan IPA

Journal of Research in Science Education

http://jppipa.unram.ac.id/index.php/jppipa/index

Mechanical Properties of Nickel, Palladium, and Platinum Nanowires: A Molecular Dynamics Study

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Received: October 8, 2024
Revised: November 30, 2024
Accepted: December 25, 2024
Published: December 31, 2024

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DOI: 10.29303/jppipa.v10i12.9667

Abstract: Transition metal group 10 nanowires exhibit exceptional mechanical properties, particularly those with FCC structures, making them promising candidates for electromechanical devices. This study used classical MD simulations with EAM potentials to explore the mechanical behavior of nickel, palladium, and platinum nanowires with varying diameters. Our findings reveal a strong correlation between nanowire diameter and mechanical properties. Increasing diameter reduces surface effects, leading to higher tensile strength. Deformation mechanisms are complex, involving phase transformations such as FCC to HCP and BCC. These results will contribute to the fundamental understanding of nanoscale mechanics and pave the way for the design of advanced nanodevices.

Keywords: Mechanical Properties; Molecular Dynamics; Nanowire

Introduction

Advancements in nanotechnology, particularly within the semiconductor industry, have led to the creation of increasingly smaller devices through the characterization and manipulation of materials at the nanoscale (Benelmekki, 2019) Various techniques for synthesizing and forming one-dimensional nanostructures exist; however, only a few have been extensively studied, including spontaneous growth, template-based synthesis, electrospinning, and lithography (Cao & Wang, 2011)

Nickel, palladium, and platinum, which belong to Group 10 of the transition metals, are utilized in numerous applications such as decoration, catalysis, superconductivity, electrical components, and alloys. Nickel is the seventh most abundant transition metal and the 22nd most prevalent element in the Earth's crust, with an abundance of 99 parts per million (ppm). In contrast, palladium and platinum are much rarer, with abundances of about 0.015 ppm and 0.01 ppm, respectively, highlighting their significant value and importance in nanotechnology (Greenwood & Earnshaw, 1997)

Research by (Aish & Starostenkov, 2016) examined the mechanical properties of metallic nanowires using a tight-binding model and molecular dynamics simulations. Their study focused on nickel nanowires, which were subjected to uniaxial tensile loading at temperatures ranging from 100 K to 1500 K. The results showed a decrease in tensile strength as temperature increased and indicated that the location of fracture depended on temperature.

In a separate study, (Y.-H. Wen, Huang, Zhu, & Wang, 2012) performed an atomistic investigation into the mechanical properties of single-crystal and five-fold twinned platinum nanowires using molecular dynamics simulations. Uniaxial tensile tests revealed that the five-fold twinned nanowire exhibited higher yield strength, but lower ductility compared to the single-crystal structure. The elastic modulus was calculated based on the deformation behavior of the nanowires using classical elasticity theory.

(Lao & Moldovan, 2008) employed the embedded-atom method (E.A.M.) potential in molecular dynamics

How to Cite:
Pamungkas, M. A., Farista, F. S., Mafazah, R., & Hidayat, A. (2024). Mechanical Properties of Nickel, Palladium, and Platinum Nanowires: A Molecular Dynamics Study. *Jurnal Penelitian Pendidikan IPA*, *10*(12), 11312–11318. https://doi.org/10.29303/jppipa.v10i12.9667

simulations to investigate the tensile behavior of palladium nanowires. The study found a spontaneous phase transformation from the face-centered cubic (F.C.C.) structure to the body-centered cubic (B.C.C.) structure at temperatures exceeding a critical threshold of 22.5 K, driven by surface tension effects.

While the mechanical properties of individual nickel, palladium, and platinum nanowires have been extensively studied, a comprehensive comparative study of these three noble metal nanowires has yet to be reported. This study employs molecular dynamics simulations using the Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) (Plimpton, 1995; Thompson et al., 2022) to investigate the deformation behavior of nickel, palladium, and platinum nanowires with varying diameters. The primary objectives are to determine the influence of diameter on maximum tensile stress and elucidate the deformation mechanisms of these noble metal nanowires under tensile loading. This research is crucial for advancing our understanding of the mechanical properties of these nanomaterials, as the findings will provide valuable insights into their deformation behavior and serve as a benchmark for future studies on nanowires with different dimensions.

Method

In this study, molecular dynamics simulations were conducted using the LAMMPS (Plimpton, 1995; Thompson et al., 2022) program, as illustrated in Figure 1.

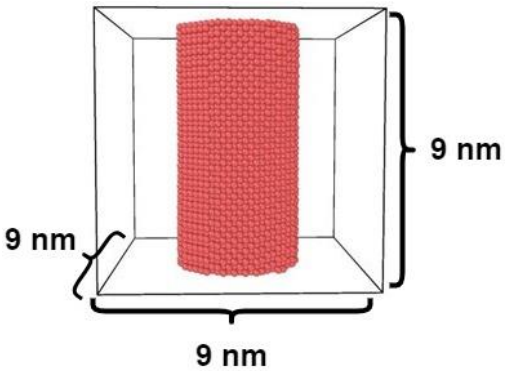


Figure 1. Dimension of Nanowire

The simulations were conducted at a constant temperature of 300 K to replicate room-temperature conditions. A velocity ranges from 10^{-3} to 10^{-13} Å/ps was selected, with an optimal value of 0.1 Å/ps. Given the metallic nature of the materials, we used the potential of an embedded atom model (EAM)*(Daw & Baskes, 1984; Daw, Foiles, & Baskes, 1993)*. A typical neighbor distance of 0.3 Å was employed for the metals. We chose the canonical (NVT) ensemble, maintaining a constant temperature while allowing for variable energy.

The materials investigated included nickel, palladium, and platinum, all characterized by a face-centered cubic (FCC) structure with specific lattice parameters: α_{Ni} = 3.52 Å, α_{Pd} = 3.89 Å, and α_{Pt} = 3.92 Å, respectively. The diameters of the nanowires ranged from 30 nm to 50 nm, with the minimum diameter set at 30 nm, as this consistently yielded well-formed nanowires in the simulations. This approach enabled subsequent tensile test analysis of the Common Neighbor Atom (CNA), visualization results in the tensile test, and their correlation with diameter using the Open Visualization Tool (OVITO).(Stukowski, 2009)

Result and Discussion

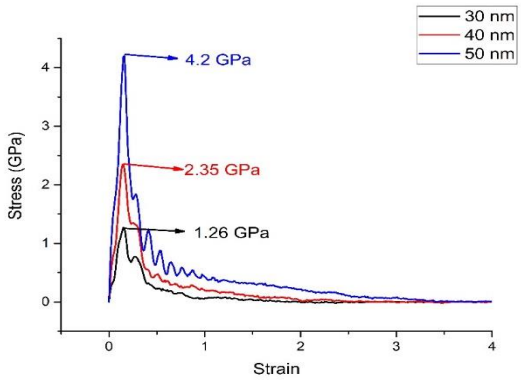


Figure 2. Stress-strain curves of nickel nanowires with diameters of 30, 40, and 50 nm

As depicted in Figure 2, the tensile strength of nickel nanowires increases with diameter, reaching a maximum of 4.2 GPa at 50 nm. Conversely, Young's modulus exhibits a more complex trend, with values of 109.49 GPa for 30 nm, 109.41 GPa for 40 nm, and 152.85 GPa for 50 nm diameters. While showing an overall trend of increasing strength with diameter, these results deviate from previous experimental studies (Budrovic, Van Swygenhoven, Derlet, Van Petegem, & Schmitt, 2004), which reported a lower tensile strength of 2.25 GPa. This discrepancy can be attributed to the presence of defects such as dislocations and voids in experimental samples, which can significantly influence the deformation behavior, as suggested by (Wang, Shan, & Huang, 2017). In contrast, simulations by (Y. H. Wen, Zhu, Shao, & Zhu, 2005) predicted a higher tensile strength of 8.62 GPa, likely due to the absence of such defects in the simulated structures.

The stress-strain curves obtained in this study exhibit a non-linear behavior characterized by a zigzag pattern, consistent with previous studies by (Y. H. Wen, Huang, Zhu, & Wang, 2012). Young's modulus values of 188.7 (Y. H. Wen et al., 2012) and 80.6 GPa (Y. H. Wen et

al., 2005) for nickel nanowires vary significantly, indicating a strong dependence on simulation parameters such as potential and diameter. The strengthening effect observed with increasing diameter can be attributed to the reduced influence of surface effects and the increasing dominance of the bulk material behavior. The presence of defects in experimental samples, as highlighted by (Seo et al., 2013) can significantly impact the mechanical properties of nanowires, with defect-free nanowires exhibiting superplastic behavior.

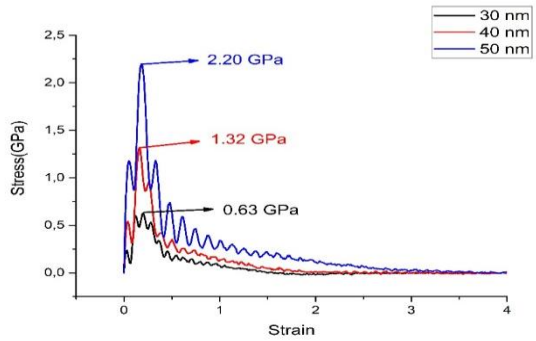


Figure 3. Stress-strain curves of palladium nanowires with diameters of 30, 40, and 50 nm

The tensile strength of palladium nanowires, as illustrated in Figure 3, shows a positive correlation with increasing diameter, peaking at 2.2 GPa for 50 nm diameters, compared to only 0.63 GPa for 30 nm. In contrast, Young's modulus exhibits an inverse correlation with diameter, decreasing from 111.84 GPa at 30 nm to 51.58 GPa at 50 nm. These results differ from those that (Y. H. Wen et al., 2012) reported, who found Young's modulus for platinum nanowires to be 181.1 GPa. The decline in Young's modulus with increasing diameter indicates that size effects significantly impact the mechanical properties of palladium nanowires. The difference between our findings and those of previous studies may be due to variations in material, simulation parameters, and the dimensions of the nanowires. The observed trends can be explained by the influence of surface effects on the inhomogeneity of the nanowire's cross-section, as predicted by (Hasmy & Medina, 2002; Wu, 2006)

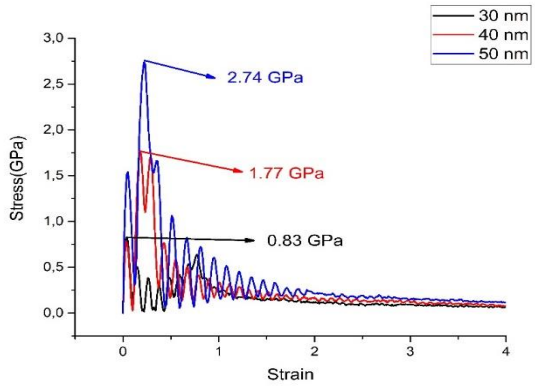
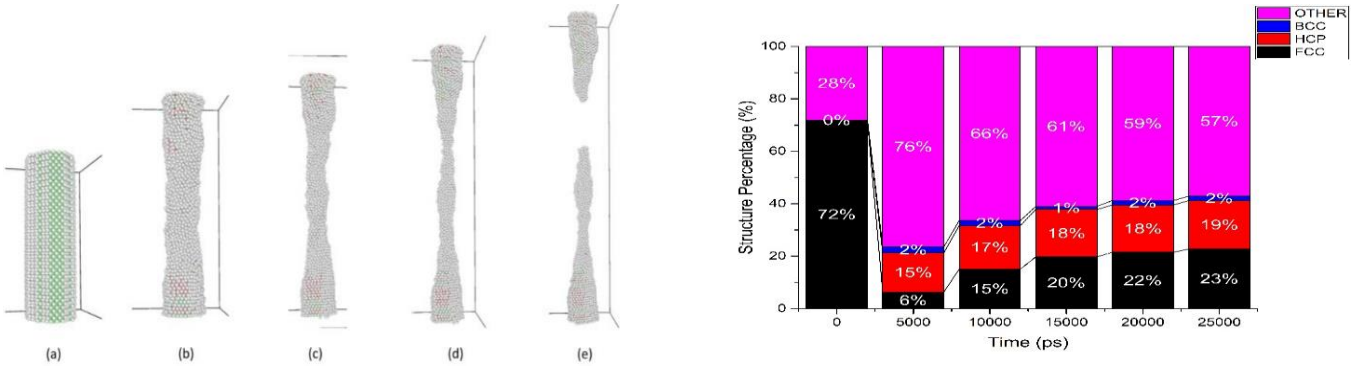


Figure 4. Stress-strain curves of platinum nanowires with diameters of 30, 40, and 50 nm

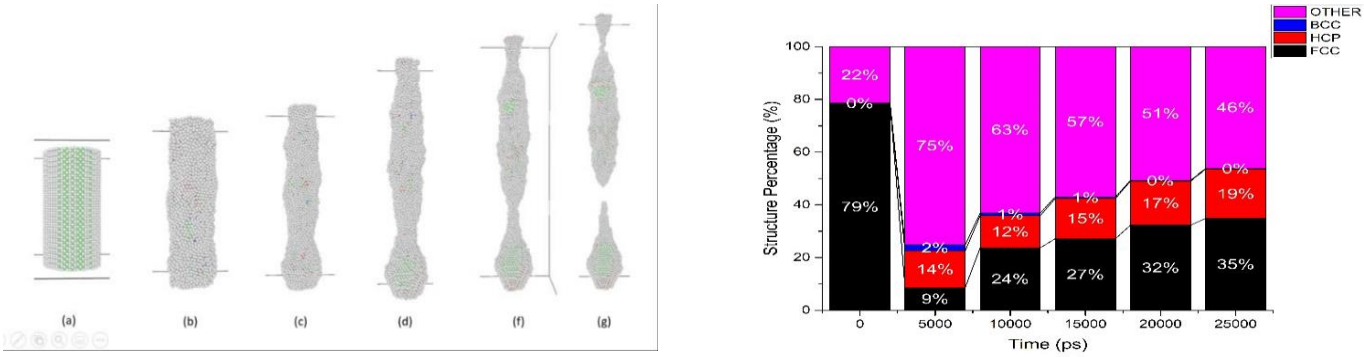
As shown in Figure 4, the tensile strength of platinum nanowires increases with diameter, reaching a maximum of 2.74 GPa at a diameter of 50 nm. In contrast, Young's modulus demonstrates a non-monotonic trend, peaking at 109.49 GPa for a diameter of 40 nm. These findings differ from earlier research by (Y. H. Wen et al., 2012) which reported a Young's modulus of 238.5 GPa for platinum nanowires.

The size-dependent mechanical behavior of metal nanowires is apparent. While Young's modulus decreases, the yield strength increases as the diameter grows. This trend is particularly noticeable for nanowires with diameters below 10 nm, where surface effects dominate. As the diameter increases, the mechanical properties tend to converge toward bulk values. This size-dependent behavior can be attributed to the increasing ratio of surface atoms to bulk atoms, which significantly influences the overall mechanical response of the nanowire. The surface atoms, extending beyond the outermost layer, play a crucial role in determining nanowires' mechanical properties, as (Wu, 2006) reported.



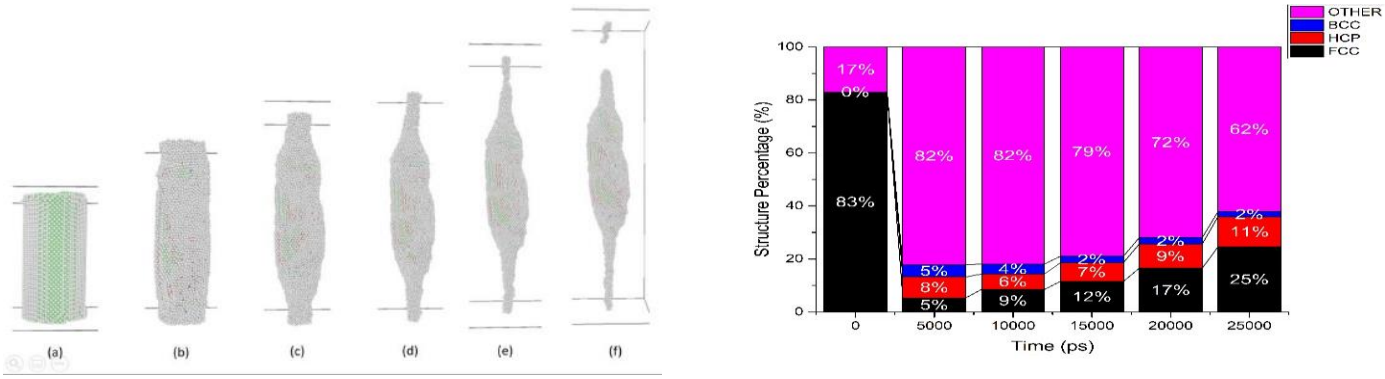
(a) (b)

Figure 5. Simulation results from 0 to 25 fs on nickel nanowires with a diameter of 30 nm: a) tensile test simulation, b) structural percentage.



(a) (b)

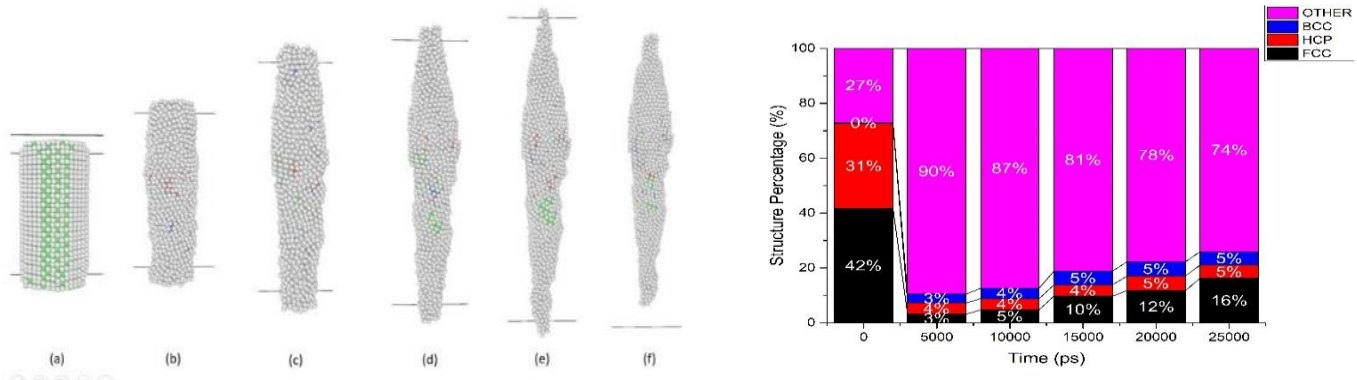
Figure 6. Simulation results from 0 to 25 fs on nickel nanowires with a diameter of 40 nm: a) tensile test simulation, b) structural percentage.



(a) (b)

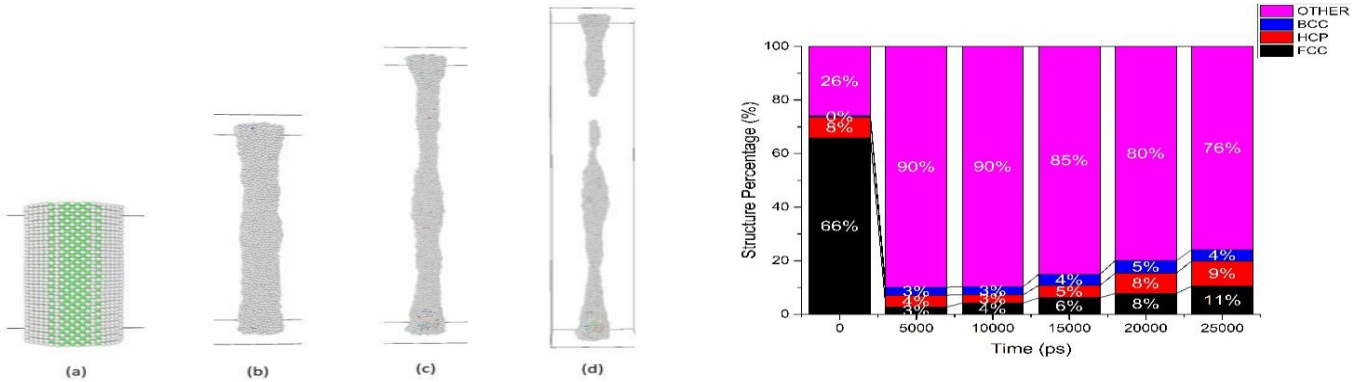
Figure 7. Simulation results from 0 to 25 fs on nickel nanowires with a diameter of 50 nm: a) tensile test simulation, b) structural percentage.

Figures 5, 6, and 7 illustrate a correlation between increasing diameter and enhanced mechanical strength in nickel nanowires. This enhancement is attributed to the increasing prevalence of the face-centered cubic (FCC) structure within the nanowires, as determined by Common Neighbor Analysis (CNA). The 50 nm diameter nanowire exhibited the highest percentage of FCC structure at 82%. However, a phase transformation from the FCC structure to a mixture of body-centered cubic (BCC), hexagonal close-packed (HCP), and other structures was observed under tensile loading. These findings align with the work of (Y. H. Wen et al., 2005), who reported the coexistence of FCC, BCC, and other structures during the tensile deformation of nickel nanowires. Consequently, it can be inferred that the initial FCC structure undergoes deformation-induced phase transformations to BCC, HCP, and other structures.



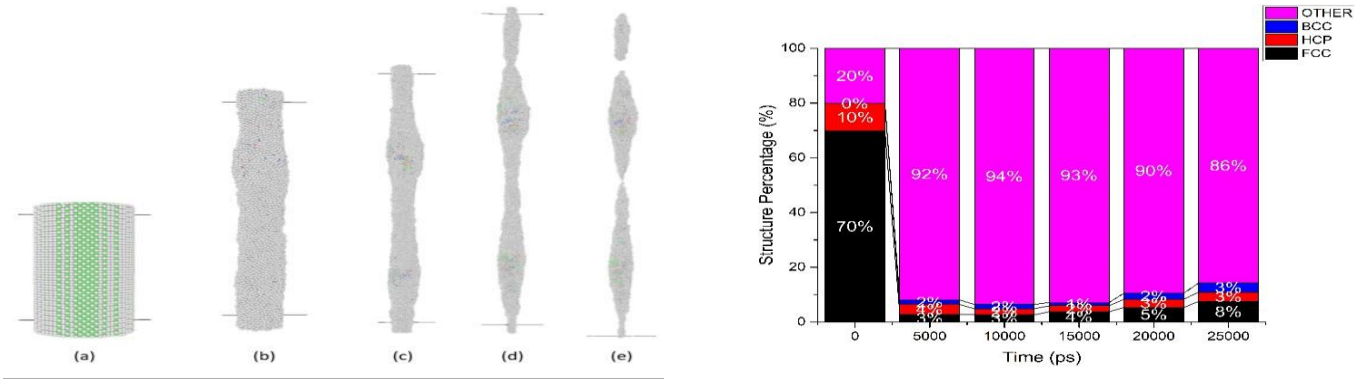
(a) (b)

Figure 8. Simulation results from 0 to 25 fs on palladium nanowires with a diameter of 30 nm: a) tensile test simulation, b) structural percentage.



(a) (b)

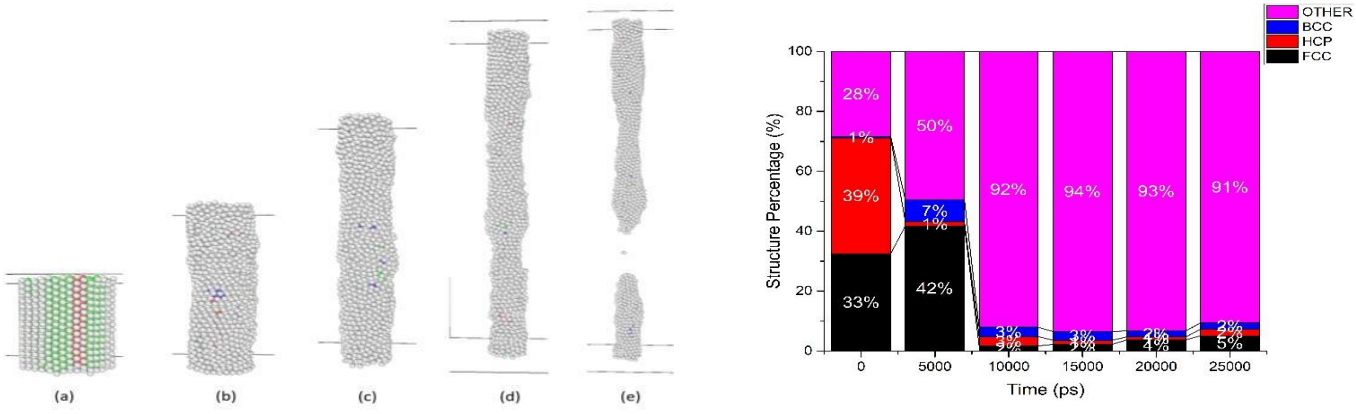
Figure 9. Simulation results from 0 to 25 fs on palladium nanowires with a diameter of 40 nm: a) tensile test simulation, b) structural percentage.



(a) (b)

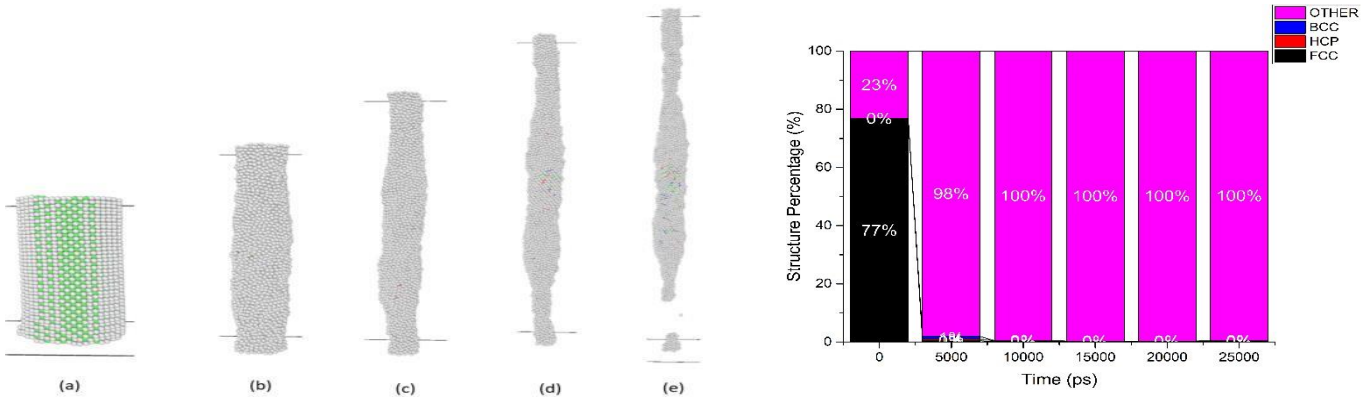
Figure 10. Simulation results from 0 to 25 fs on palladium nanowires with a diameter of 50 nm: a) tensile test simulation, b) structural percentage.

The analysis of palladium nanowires with varying diameters (Figures 8-10) reveals a direct correlation between diameter and mechanical strength. This correlation is attributed to the increasing proportion of face-centered cubic (FCC) and hexagonal close-packed (HCP) structures within the nanowires, as determined by Common Neighbor Analysis (CNA). The 50 nm diameter nanowire exhibited the highest percentage of these structures. However, tensile testing induced a phase transformation from the initial FCC structure to a mixture of BCC, HCP, and other structures. The observed trends can be explained by the influence of surface effects on the inhomogeneity of the nanowire's cross-section, as predicted by (Hasmy & Medina, 2002; Wu, 2006).



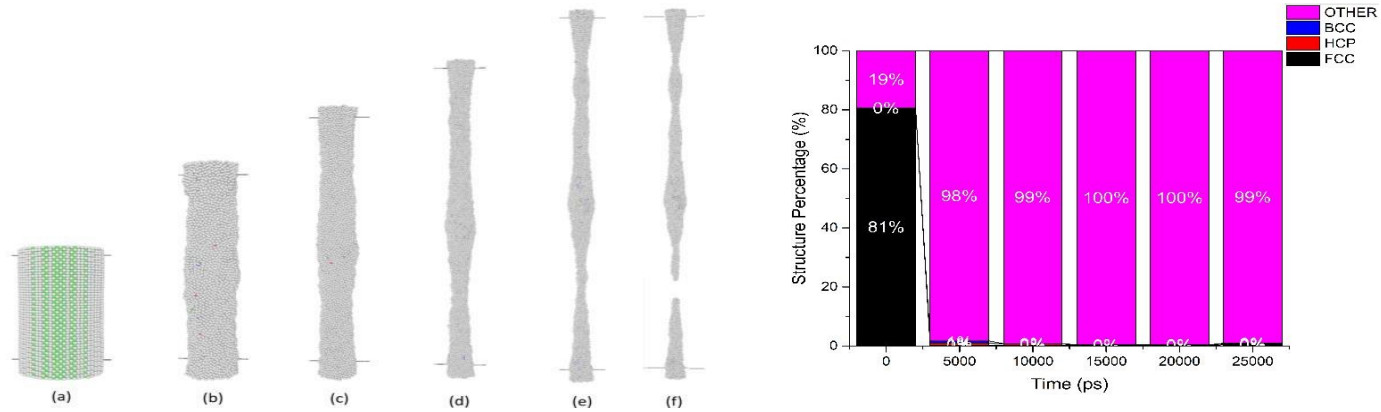
(a) (b)

Figure 11. Simulation results from 0 to 25 fs on platinum nanowires with a diameter of 30 nm: a) tensile test simulation, b) structural percentage.



(a) (b)

Figure 12. Simulation results from 0 to 25 fs on platinum nanowires with a diameter of 40 nm: a) tensile test simulation, b) structural percentage.



(a) (b)

Figure 13. Simulation results from 0 to 25 fs on platinum nanowires with a diameter of 50 nm: a) tensile test simulation, b) structural percentage.

The analysis of platinum nanowires with varying diameters (Figures 11-13) reveals a direct correlation between diameter and mechanical strength. This correlation is attributed to the increasing proportion of face-centered cubic (FCC) structures within the nanowires, as determined by Common Neighbor Analysis (CNA). The 50 nm diameter nanowire exhibited the highest percentage of FCC structure. However, tensile testing induced a phase transformation from the initial FCC structure to a mixture of BCC, HCP, and other structures. This size-dependent behavior can be attributed to the increasing ratio of surface atoms to bulk atoms, which significantly influences the overall mechanical response of the nanowire. The surface atoms, extending beyond the outermost layer, play a crucial role in determining nanowires' mechanical properties, as (Wu, 2006) reported.

Conclusion

The findings suggest that diameter significantly influences the mechanical properties of nanowires. The 50 nm nickel nanowire displayed the highest tensile strength and Young's modulus, while the 30 nm platinum nanowire exhibited the lowest. The increase in tensile strength with diameter can be attributed to the reduced influence of surface effects and the increasing dominance of the bulk material behavior. The observed structural transformations from FCC to HCP, BCC, and other structures during deformation support the notion that the deformation mechanism is complex and involves phase transformations.

Acknowledgments
We would like to acknowledge support provided by Universitas Brawijaya

Author Contributions
Conceptualization, M.A.; methodology, M.A.; software, R.M; validation: F.S.; formal analysis, M.A.; investigation, F.S.; data curation, R.M.; writing—original draft preparation, R.M.; writing—review and editing, F.S.; visualization, F.S and R.M.; supervision: M.A and A.H. All authors have read and agreed to the published version of the manuscript.

Funding
This research received no external funding

Conflicts of Interest
The researchers in this study were assigned by each institution with the aim of improving the lecturers' resources.

References

Aish, M., & Starostenkov, M. (2016). Mechanical properties of metallic nanowires using tight-binding model. *AIP Conference Proceedings*, *1698*. American Institute of Physics Inc. https://doi.org/10.1063/1.4937842

Benelmekki, M. (2019). Nanomaterials. In *The original product of nanotechnology*. Morgan & Claypool Publishers. https://doi.org/10.1088/2053-2571/ab126d

Budrovic, Z., Van Swygenhoven, H., Derlet, P. M., Van Petegem, S., & Schmitt, B. (2004). Plastic Deformation with Reversible Peak Broadening in Nanocrystalline Nickel. *Science*, *304*(5668), 273–276. https://doi.org/10.1126/science.1095071

Cao, G., & Wang, Y. (2011). Nanostructures and Nanomaterials. In *World Scientific Series in Nanoscience and Nanotechnology*. WORLD SCIENTIFIC. https://doi.org/doi:10.1142/7885

Daw, M. S., & Baskes, M. I. (1984). Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. *Physical Review B*, *29*, 6443–6453.

Daw, M. S., Foiles, S. M., & Baskes, M. I. (1993). The embedded-atom method: a review of theory and applications. *Materials Science Reports*, *9*(7), 251–310. https://doi.org/https://doi.org/10.1016/0920-2307(93)90001-U

Greenwood, N. N., & Earnshaw, A. (1997). 27 - Nickel, Palladium and Platinum. In N. N. GREENWOOD & A. EARNSHAW (Eds.), *Chemistry of the Elements (Second Edition)* (pp. 1144–1172). Oxford: Butterworth-Heinemann. https://doi.org/https://doi.org/10.1016/B978-0-7506-3365-9.50033-X

Hasmy, A., & Medina, E. (2002). Thickness Induced Structural Transition in Suspended fcc Metal Nanofilms. *Physical Review Letters*, *88*(9), 96103. https://doi.org/10.1103/PhysRevLett.88.096103

Lao, J., & Moldovan, D. (2008). Surface stress induced structural transformations and pseudoelastic effects in palladium nanowires. *Applied Physics Letters*, *93*(9), 093108. https://doi.org/10.1063/1.2976434

Plimpton, S. (1995). Fast Parallel Algorithms for Short-Range Molecular Dynamics. *Journal of Computational Physics*, *117*(1), 1–19. https://doi.org/https://doi.org/10.1006/jcph.1995.1039

Seo, J.-H., Park, H. S., Yoo, Y., Seong, T.-Y., Li, J., Ahn, J.-P., … Choi, I.-S. (2013). Origin of Size Dependency in Coherent-Twin-Propagation-Mediated Tensile Deformation of Noble Metal Nanowires. *Nano Letters*, *13*(11), 5112–5116. https://doi.org/10.1021/nl402282n

Stukowski, A. (2009). Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *Modelling and Simulation in Materials Science and Engineering*, *18*(1), 15012. https://doi.org/10.1088/0965-0393/18/1/015012

Thompson, A. P., Aktulga, H. M., Berger, R., Bolintineanu, D. S., Brown, W. M., Crozier, P. S., … Plimpton, S. J. (2022). LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications*, *271*. https://doi.org/10.1016/j.cpc.2021.108171

Wang, S., Shan, Z., & Huang, H. (2017). The Mechanical Properties of Nanowires. *Advanced Science*, *4*(4), 1600332. https://doi.org/https://doi.org/10.1002/advs.201600332

Wen, Y. H., Huang, R., Zhu, Z. Z., & Wang, Q. (2012). Mechanical properties of platinum nanowires: An atomistic investigation on single-crystalline and twinned structures. *Computational Materials Science*, *55*, 205–210. https://doi.org/10.1016/j.commatsci.2011.11.020

Wen, Y. H., Zhu, Z. Z., Shao, G. F., & Zhu, R. Z. (2005). The uniaxial tensile deformation of Ni nanowire: Atomic-scale computer simulations. *Physica E: Low-Dimensional Systems and Nanostructures*, *27*(1–2), 113–120. https://doi.org/10.1016/j.physe.2004.10.009

Wen, Y.-H., Huang, R., Zhu, Z.-Z., & Wang, Q. (2012). Mechanical properties of platinum nanowires: An atomistic investigation on single-crystalline and twinned structures. *Computational Materials Science*, *55*, 205–210. https://doi.org/https://doi.org/10.1016/j.commatsci.2011.11.020

Wu, H. A. (2006). Molecular dynamics study on mechanics of metal nanowire. *Mechanics Research Communications*, *33*(1), 9–16. https://doi.org/https://doi.org/10.1016/j.mechrescom.2005.05.012