

O. Palchekovskyi, A. Orlov, Yu. Yavorskyi, I. Kruhlov

Tensile Deformation of Ni/Ti Multilayers: Coupled Effects of Modulation Period and Strain Rate from Molecular Dynamics Simulations

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, Ukraine, yu.yavorskyi@kpi.ua

The mechanical response of Ni/Ti multilayers is governed by the interplay between interface-mediated deformation and structural transformations in the constituent layers. Here, molecular dynamics simulations are used to investigate the tensile deformation of planar Ni/Ti multilayers with modulation periods of 28.6 nm – 9.5 nm over strain rates of 10^8 s^{-1} – 10^{10} s^{-1} . Decreasing the modulation period reduces the tensile strength by ~8% and substantially modifies the post-yield deformation, including the partitioning of dislocation activity between the Ni and Ti layers and the formation and persistence of deformation-induced BCC Ti. Increasing the strain rate has a comparatively weak effect on tensile strength but systematically delays the structural transformations. Pronounced stacking faults in Ni develop at ~8% strain at 10^8 s^{-1} but only at ~13% at 10^{10} s^{-1} . At the highest strain rate, the HCP-to-BCC transformation in Ti is also delayed and becomes more abrupt, producing finer and more dispersed BCC regions. Overall, the results show that the modulation period primarily determines the deformation pathway and distribution of plasticity between the constituent layers, whereas the strain rate primarily controls the onset and kinetics of the deformation processes.

Keywords: Molecular Dynamics, Modulation Periods, Uniaxial Tension, Mechanical Properties, Ni/Ti Multilayers, Dislocation Density.

Received 26 April 2026; Accepted 20 September 2026; Published 30 September 2026.

Introduction

Ni/Ti multilayers are of considerable technological and fundamental interest. They provide a convenient precursor architecture for functional NiTi thin films used in MEMS/NEMS actuators, sensors, microvalves, micropumps, and related devices [1]. The multilayer route enables composition control through the individual Ni and Ti layer thicknesses, followed by thermally activated interdiffusion and intermetallic phase formation [2-4]. At the same time, the large negative Gibbs free energy of mixing and asymmetric atomic mobility of Ni and Ti promote interfacial mixing and solid-state amorphization, whose extent is strongly affected by the modulation period and interface density [5-8].

For practical MEMS/NEMS applications, the mechanical stability of such systems is equally important. Thin-film actuators and sensors operate under repeated or

transient mechanical loading, with TiNi films capable of generating large recoverable transformation strains and stresses [1]. Their performance and reliability therefore depend strongly on fatigue resistance and the stability of the underlying deformation mechanisms. In nanoscale multilayers, these properties are governed not only by the intrinsic response of the constituent metals but also by interface-mediated dislocation processes and deformation-induced structural transformations.

Direct experimental observation of these processes at the atomic scale is difficult, particularly within individual nanometer-thick layers. Molecular dynamics (MD) simulations therefore provide a powerful complementary approach, enabling direct analysis of local strain, dislocation activity, and phase transformations during deformation. Atomistic studies of metallic multilayers have demonstrated a strong dependence of their mechanical response on interface structure, characteristic

layer thickness, and loading conditions. In Cu/Ta multilayers, variations in the modulation period and interface structure were found to affect dislocation nucleation and propagation and the resulting tensile response [9], while simulations performed at different strain rates revealed corresponding changes in the stress-strain behavior, dislocation evolution, and structural transformations [10]. In Ni/Co multilayers, the effects of layer thickness and strain rate were associated with changes in interface-mediated dislocation activity and stacking-fault formation [11]. For Ti-containing systems, an additional factor is the structural instability of nanoscale Ti: decreasing the Ti layer thickness can stabilize metastable body-centered cubic (BCC) Ti in Ti/V and Ti/Ta multilayers [12–13], while simulations of hexagonal close-packed (HCP) Ti have shown deformation-induced transformations involving intermediate BCC configurations [14]. A study of Ti/Ni multilayered nanowires further demonstrated that layer thickness and strain rate can jointly affect tensile strength and the dominant deformation mechanisms [15]. However, considerably less is known about how these two factors interact in planar Ni/Ti multilayers, where deformation is governed by the response of the individual Ni and Ti layers and their interfaces rather than by the pronounced free-surface effects inherent to nanowires. In particular, it remains unclear how changes in modulation period and strain rate affect the balance between dislocation-mediated plasticity and deformation-induced structural transformations and, consequently, the overall mechanical response of the multilayer.

In the present work, MD simulations performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) are employed to systematically investigate the coupled effects of modulation period and strain rate on the tensile deformation of planar Ni/Ti multilayers. Three modulation periods are examined over strain rates ranging from 10^8 s^{-1} to 10^{10} s^{-1} . The mechanical response is correlated with atomic-scale structural evolution, phase fractions, local von Mises shear strain, and layer-resolved dislocation density to determine how interface density and loading rate govern phase transformations, strain localization, and the partitioning of plastic deformation between the Ni and Ti layers.

I. Simulation methodology

The initial atomistic models of the Ni/Ti multilayer films were constructed using the Atoms tool [16] (Fig. 1). The interfacial boundaries were created by joining the close-packed planes of both phases along the z -axis (the film growth direction), specifically matching face-centered cubic (FCC) Ni(111) with HCP Ti(0001). The in-plane crystallographic orientations were aligned as $\text{Ni}[1\bar{1}0] \parallel \text{Ti}[2\bar{1}\bar{1}0]$ along the x -axis, and $\text{Ni}[11\bar{2}] \parallel \text{Ti}[01\bar{1}0]$ along the y -axis, matching the classic orientation relationship for FCC/HCP systems. To minimize initial artificial structural misfit strains at the phase boundaries, commensurate supercells were constructed by matching 120 and 101 unit cells of Ni and Ti along the x -axis, and 7 and 6 unit cells along the y -axis, respectively. The overall dimensions of the computational domains are

approximately $30 \text{ nm} \times 3 \text{ nm} \times 28.6 \text{ nm}$.

To systematically investigate the influence of interface density, three configurations were generated: bi-layer, four-layer, and six-layer films. All models maintained a constant total thickness of 28.6 nm and contained precisely 193,680 atoms. The corresponding modulation periods (Δ), defined as the thickness of a single Ni/Ti bilayer, are $\Delta_1 = 28.6 \text{ nm}$ (bi-layer), $\Delta_2 = 14.3 \text{ nm}$ (four-layer), and $\Delta_3 = 9.5 \text{ nm}$ (six-layer), respectively.

All molecular dynamics (MD) simulations were carried out using the open-source Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [17]. The interatomic interactions in the Ni-Ti system were described using the second nearest-neighbor modified embedded-atom method (2NN-MEAM) potential developed by Kim et al. [18]. This potential was selected for its proven accuracy in reproducing the structural, elastic, and thermodynamic properties of the Ni-Ti system, as well as its ability to capture phase stability at finite temperatures.

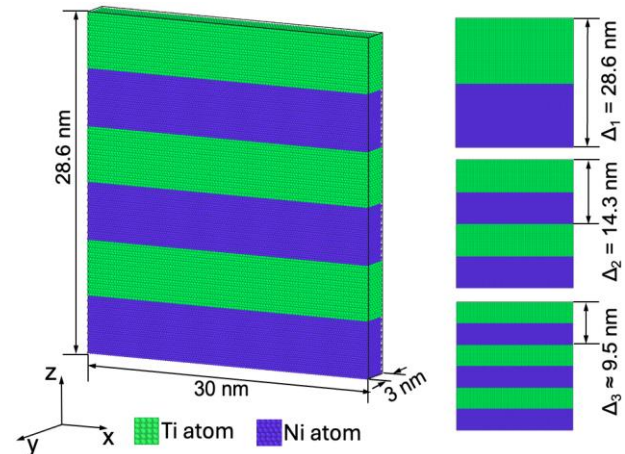


Fig. 1. Simulation models of the Ni/Ti multilayer films with different Δ of 28.6 nm, 14.3 nm, and 9.5 nm.

Given that the object of study is a freestanding thin film, periodic boundary conditions were applied along the in-plane x and y directions, while non-periodic, shrink-wrapped boundary conditions were imposed along the z -axis (the film growth direction). Before the mechanical testing, each model underwent a strict equilibration procedure to relieve initial structural misfit strains at the phase boundaries and achieve a stable thermodynamic state. Initially, a static energy minimization was performed using the conjugate gradient algorithm. Subsequently, the sample was dynamically equilibrated for 100 ps at 300 K under an isothermal-isobaric (NPT) ensemble. During this relaxation phase, the Nose-Hoover pressure barostat was configured to maintain zero pressure strictly in both periodic in-plane directions (x and y axes). The time step for all dynamic integrations was set to 2 fs [10–11, 19].

Following equilibration, uniaxial tensile tests were simulated by applying a continuous affine deformation along the x -axis at constant strain rates of 10^8 s^{-1} , $5 \cdot 10^8 \text{ s}^{-1}$, 10^9 s^{-1} , $5 \cdot 10^9 \text{ s}^{-1}$, and 10^{10} s^{-1} . During the tension process, the NPT ensemble was maintained at 300 K, but the pressure barostat was coupled exclusively to the

transverse y-axis to maintain zero stress, thereby correctly capturing the Poisson effect while the z-axis deformed freely into the vacuum. The engineering strain was calculated as $\Delta L_x/L_{x0}$, and the corresponding engineering stress was derived directly from the global pressure tensor component (P_{xx}), which accounts for the actual film volume due to the tightly shrink-wrapped boundaries along the z-axis.

The OVITO software was adopted to visualize the evolution of the atomic structure and analyze the deformation mechanisms [20]. The local crystalline structure and phase transitions at the interfaces were identified using the Common Neighbor Analysis (CNA), while the Dislocation Extraction Algorithm (DXA) tool was applied to compute the dislocation density during the tensile loading.

II. Results & Discussion

Figure 2 summarizes the tensile response of the Ni/Ti multilayers with different modulation periods at a strain rate of 10^9 s^{-1} . Figure 2(a) shows the corresponding stress-strain curves, which exhibit similar patterns and can be divided into three characteristic stages: elastic

deformation (*Stage I*), rapid stress decrease (*Stage II*), and post-yield deformation (*Stage III*).

In *Stage I*, the stress increases approximately linearly with strain and reaches its maximum at a strain of approximately 0.08. Young's modulus, determined from the linear portion of the stress-strain curves, is nearly independent of the modulation period and amounts to $140 \pm 4 \text{ GPa}$. After reaching the maximum, the stress rapidly decreases in *Stage II*. In *Stage III*, the stress partially recovers and subsequently fluctuates with increasing strain. Figure 2(b) shows that the tensile strength (defined as the maximum stress reached in *Stage I*) decreases with decreasing modulation period, from approximately 10.28 GPa at Δ_1 to 9.76 GPa at Δ_2 and 9.49 GPa at Δ_3 . Thus, reducing the modulation period from 28.6 nm (Δ_1) to 9.5 nm (Δ_2) results in a decrease in tensile strength of approximately 7.7%.

Figure 3 shows the structural evolution of the Ni/Ti multilayers with different Δ at selected strains representing the characteristic regions of the stress-strain response in Fig. 2(a). At 6% strain (*Stage I*), the initial HCP structure of Ti and FCC structure of Ni are largely preserved for all three modulation periods. The onset of structural transformations is observed at 8% strain, immediately after the transition from *Stage I* to *Stage II*,

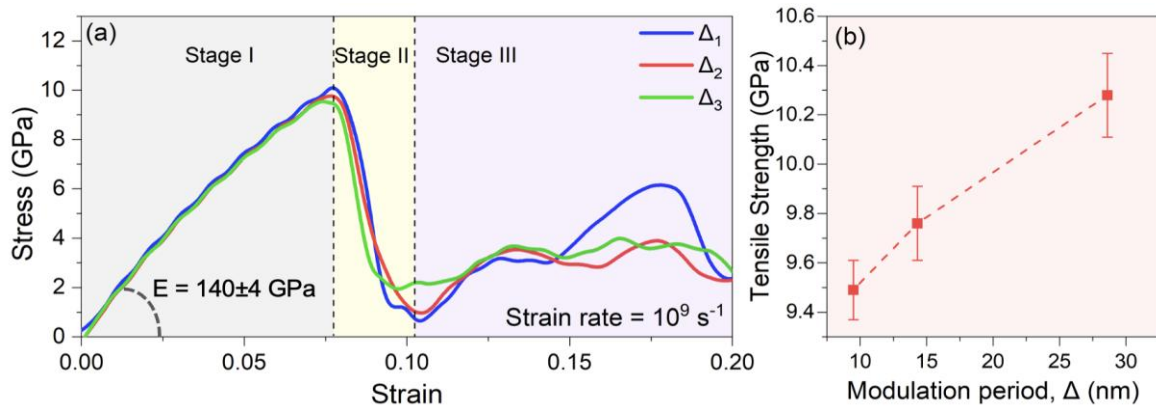


Fig. 2. (a) Stress-strain curves for the Ni/Ti multilayers at a strain rate of 10^9 s^{-1} ; (b) Dependence of the tensile strength on the Δ .

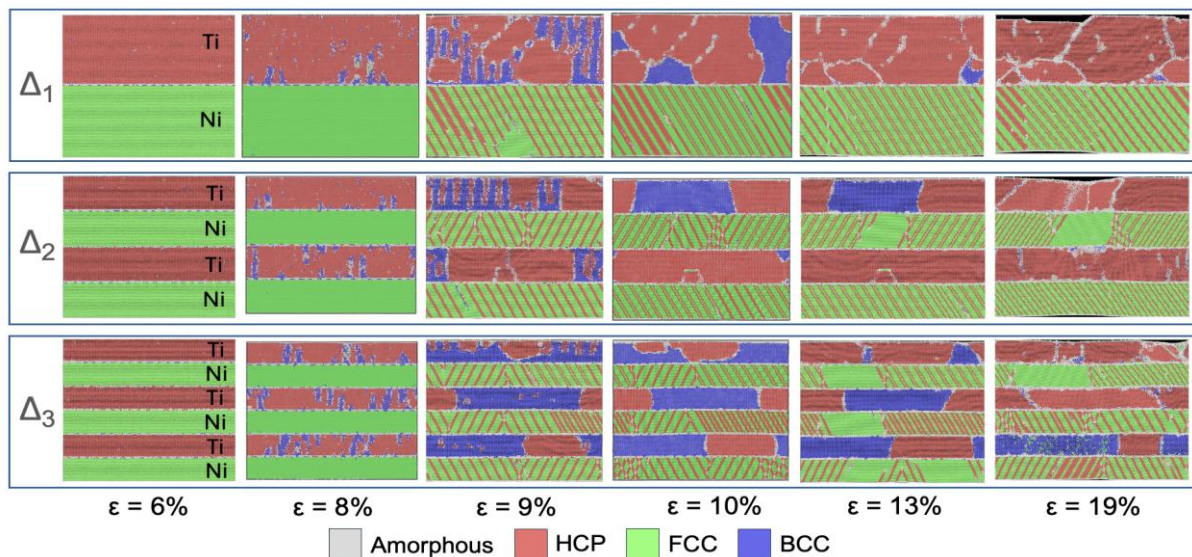


Fig. 3. Structural evolution of the Ni/Ti multilayers at tensile strains of 6%, 8%, 9%, 10%, 13%, and 19% at a strain rate of 10^9 s^{-1} .

with the appearance of BCC regions within the initially HCP Ti layers and HCP regions within the initially FCC Ni layers. By 9% strain, these transformations become pronounced, with extensive BCC regions developing in Ti and inclined stacking faults forming within the FCC Ni layers. With further deformation, the structural evolution becomes increasingly dependent on the modulation period. For Δ_1 , the Ti layers remain predominantly HCP, with BCC regions appearing only locally, whereas decreasing Δ promotes more extensive and persistent BCC regions, particularly for Δ_3 . This difference remains evident at higher strains: at 19%, the Ti layers are predominantly HCP for Δ_1 and Δ_2 , while substantial BCC regions persist for Δ_3 . This behavior can be associated with the increasing interfacial contribution at smaller modulation periods, since reduced Ti layer thickness has been shown to promote the stabilization of metastable BCC Ti in nanoscale multilayers [12–13], while deformation-induced BCC Ti may transform back to HCP upon further straining [14]. In contrast, the Ni layers exhibit a broadly similar evolution for all three modulation periods, characterized by the coexistence of FCC and deformation-induced HCP regions throughout the later stages of deformation. In addition to these structural transformations, a pronounced surface step develops in the upper Ni layer of Δ_1 at 19% strain, indicating localized plastic deformation reaching the free surface.

A quantitative assessment of these structural transformations is provided by the evolution of the FCC, HCP, BCC, and amorphous phase fractions as a function of tensile strain (Fig. 4). For all modulation periods, the phase fractions change gradually during the initial loading stage, followed by a pronounced redistribution at strains of approximately 8%–9%, coinciding with the rapid stress decrease in *Stage II* (Fig. 2(a)). For Δ_1 , the BCC fraction increases sharply to approximately 25% at ~9% strain and then progressively decreases, approaching zero at ~13%, while the HCP fraction simultaneously increases to above 40%. For Δ_2 , the BCC fraction reaches a considerably lower maximum of approximately 12% and remains below 10% over most of the subsequent strain range before disappearing at ~16%. A different evolution is observed for Δ_3 , where the BCC fraction rapidly increases to approximately 30% at ~9% strain and remains close to this level up to ~13%, followed by a gradual decrease to nearly zero at ~17%. This decrease is accompanied by a pronounced recovery of the HCP fraction, consistent with the BCC-to-HCP structural rearrangement observed in the atomistic configurations. The amorphous fraction also evolves during deformation and is systematically higher for Δ_3 over most of the investigated strain range, reaching approximately 20%–25% before the onset of *Stage II* and remaining above ~15% at larger strains. Thus, the quantitative phase analysis reveals distinct transformation pathways for the three modulation periods, particularly in terms of the magnitude and persistence of the deformation-induced BCC fraction and the fraction of structurally disordered atoms.

The spatial distribution of the local von Mises shear strain provides further insight into the deformation mechanisms underlying the structural changes described above (Fig. 5). At 6% strain, the local shear strain remains

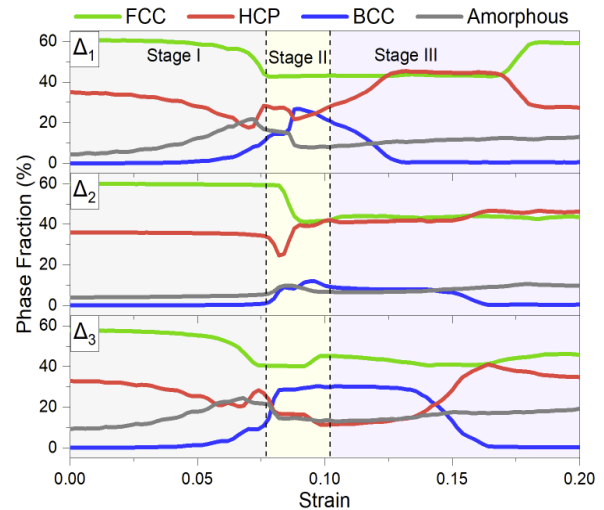


Fig. 4. Evolution of the atomic phase fractions (FCC, HCP, BCC, and amorphous) as a function of tensile strain for the Ni/Ti multilayers.

relatively low within the interiors of the Ni and Ti layers (~0.02–0.04), while regions of enhanced strain are already visible near the Ni/Ti interfaces (~0.06–0.08). At 8% strain, strain localization becomes more pronounced, with local shear strain reaching ~0.10–0.15 in regions extending from the interfaces into the adjacent layers. At 9%–10% strain, inclined bands with local shear strain of ~0.15–0.25 develop within the Ni layers and spatially correlate with the stacking faults identified from the structural analysis (Fig. 3). A similar behavior has been reported for Ni/Co multilayers, where stacking faults were found to initiate at the interfaces and subsequently propagate into the Ni layers [11]. With further deformation, the localized high-strain regions extend through both Ni and Ti layers, resulting in increasingly heterogeneous strain distributions. The effect of the modulation period becomes particularly evident at larger strains. At 19% strain, Δ_1 exhibits pronounced strain localization within several intense bands extending across the multilayer, consistent with the surface step observed in the corresponding atomic configuration, whereas Δ_2 and Δ_3 exhibit a larger number of localized high-strain regions distributed throughout the multilayer. Overall, the strain maps indicate that the Ni/Ti interfaces are preferential regions for the development of local deformation and that the subsequent pattern of strain localization varies with the modulation period.

To further clarify the mechanisms underlying the strain localization observed in Fig. 5, the evolution of the dislocation density was analyzed separately within the Ni and Ti layers (Fig. 6).

During *Stage I*, no appreciable dislocation activity is observed in either constituent for all three modulation periods. At the onset of *Stage II*, the dislocation density increases abruptly in the Ni layers for all three Δ , reaching values approximately 3–5 times higher than those in the Ti layers. This onset coincides with the formation of inclined stacking faults in Ni (Fig. 3) and the corresponding regions of elevated local shear strain (Fig. 5), indicating that the initial plastic response is primarily associated with dislocation activity in the Ni layers. During *Stage III*, the evolution of the dislocation

density differs substantially among the three modulation periods. For Δ_1 , the Ni dislocation density decreases from its initial maximum of $\sim 4 \cdot 10^{16} \text{ m}^{-2}$, whereas the density in Ti increases rapidly and remains approximately 3–4 times higher than in Ni throughout most of *Stage III*. For Δ_2 , the dislocation densities in Ni and Ti remain comparable over the first part of *Stage III*, followed by a simultaneous increase above ~ 0.16 strain, where both reach values approximately 2–3 times higher than at the beginning of the stage. In contrast, for Δ_3 , the Ni dislocation density remains approximately $2\text{--}4 \cdot 10^{16} \text{ m}^{-2}$ throughout most of *Stage III*, while dislocation activity in Ti is strongly suppressed and remains at least ~ 3 times lower up to ~ 0.17 strain, followed by a sharp increase at higher strains.

Thus, the dislocation analysis reveals a modulation-period-dependent partitioning of plastic deformation between the constituent layers, with Ti dominating the dislocation activity in Δ_1 , both constituents becoming strongly involved at high strains in Δ_2 , and Ni carrying most of the dislocation activity over the major part of *Stage III* in Δ_3 . Such a redistribution can be associated with the dual role of interfaces as preferential sites for

dislocation nucleation and barriers to their propagation, while changes in layer thickness and interface spacing modify the dislocation activity and the relative contribution of the constituent layers to plastic deformation [9; 11].

Having established the differences in deformation mechanisms associated with the modulation period at a strain rate of 10^9 s^{-1} , we next examine how the mechanical response of the Ni/Ti multilayers evolves over a broader range of strain rates (Fig. 7). For all three modulation periods, the initial portions of the stress–strain curves remain similar over the investigated strain-rate range, while the maximum tensile stress shows only a moderate increase with increasing strain rate (from $\sim 9.5\text{--}9.9 \text{ GPa}$ at 10^8 s^{-1} to $\sim 10.2\text{--}10.5 \text{ GPa}$ at 10^{10} s^{-1}). A considerably stronger rate dependence is observed in the position of the stress maximum and the subsequent rapid stress drop, which shift systematically toward higher strains as the strain rate increases from 10^8 s^{-1} to 10^{10} s^{-1} . At 10^8 s^{-1} , the stress decreases to values close to zero during the rapid relaxation stage for all three Δ ; however, the depth of the stress minimum does not exhibit a simple monotonic

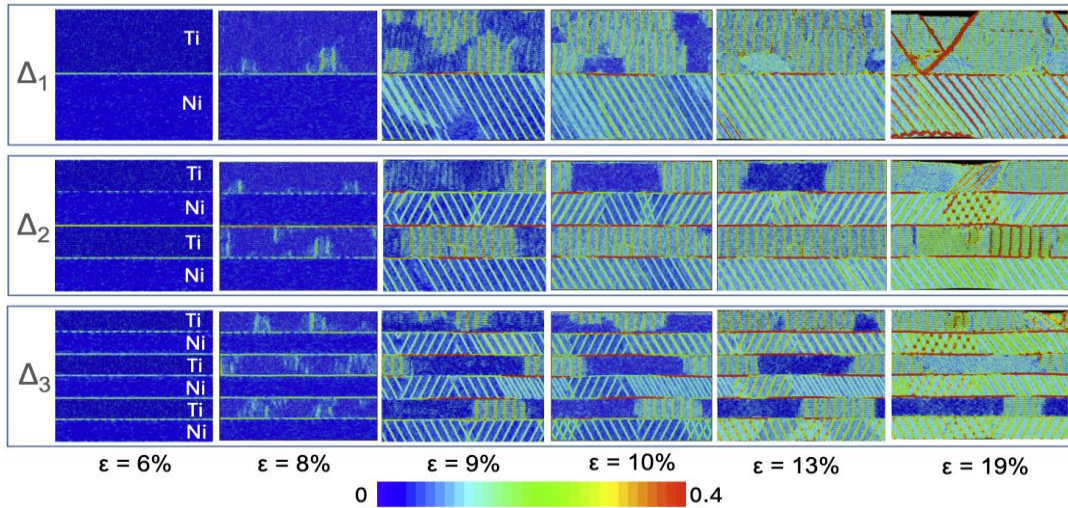


Fig. 5. Local von Mises shear strain distribution in the Ni/Ti multilayers at tensile strains of 6%, 8%, 9%, 10%, 13%, and 19% at a strain rate of 10^9 s^{-1} .

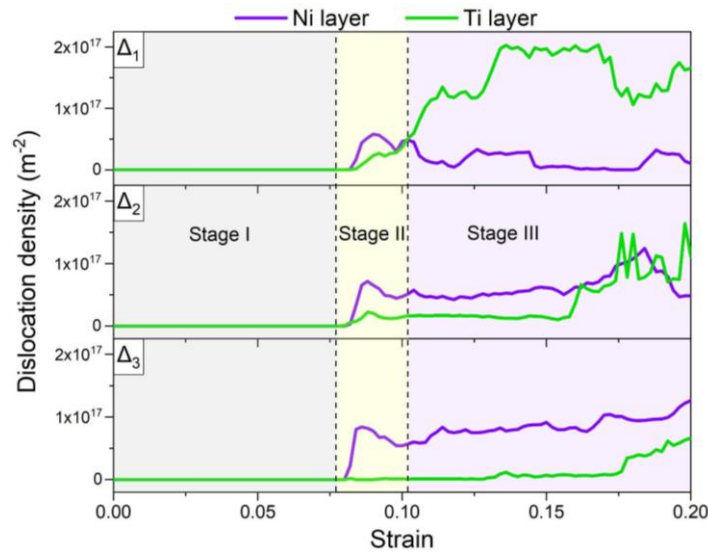


Fig. 6. Dislocation density as a function of strain within the individual Ni and Ti layers for the Ni/Ti multilayers at a strain rate of 10^9 s^{-1} .

dependence on strain rate. The main effect of increasing strain rate is a shift of the stress maximum and subsequent rapid stress drop toward higher strains. In contrast, the tensile strength changes only moderately, while no clear strain-rate dependence is observed in the post-yield region.

To evaluate the effect of strain rate on the structural evolution, the two limiting strain rates, 10^8 s^{-1} and 10^{10} s^{-1} , are compared with the results obtained at 10^9 s^{-1} (Fig. 3). At 10^8 s^{-1} (Fig. 8), structural transformations become more advanced at an earlier stage of deformation. At 8% strain, BCC regions are already well developed within the Ti layers, whereas only the initial formation of this phase is observed at 10^9 s^{-1} (Fig. 3). An even clearer strain-rate effect is observed in Ni: inclined stacking faults are already pronounced at 8% strain at 10^8 s^{-1} , while at 10^9 s^{-1} they become clearly developed only at ~9% strain. At higher strains (13–19%), the effect of modulation period follows the same general pattern as at 10^9 s^{-1} : BCC Ti is largely replaced by HCP Ti in Δ_1 and Δ_2 , whereas substantial BCC regions persist in Δ_3 up to 19% strain.

At the highest strain rate of 10^{10} s^{-1} (Fig. 9), the structural transformations are markedly delayed compared with those at lower rates (Fig. 8, Fig. 3). The Ni layers remain predominantly FCC up to ~10% strain, and pronounced inclined stacking faults appear only at ~13%, compared with ~8% at 10^8 s^{-1} (Fig. 8) and ~9% at 10^9 s^{-1} (Fig. 3). A similar delay is observed in Ti: the HCP

structure remains dominant to higher strain, followed by an abrupt HCP-to-BCC transformation in which BCC regions rapidly occupy a substantial fraction of the Ti layers. Notably, these BCC regions are considerably finer and more dispersed than those formed at lower strain rates, indicating extensive nucleation with limited subsequent growth. This strain-rate-induced delay is consistent with previous MD studies of Ni/Co and Cu/Ta multilayers, where increasing the strain rate shifted dislocation and phase-transformation onset to higher strains and reduced the time available for atomic rearrangement and stress relaxation [10–11]. At 10^{10} s^{-1} , the deformation therefore approaches an ultrahigh-rate regime in which structural relaxation is strongly constrained, resulting in delayed but more abrupt transformation and the formation of a highly dispersed BCC Ti structure.

Overall, the present results demonstrate a pronounced sensitivity of the deformation behavior of Ni/Ti multilayers to both modulation period and strain rate. The former affects the distribution of plastic deformation between the constituent layers and the stability of deformation-induced BCC Ti, whereas increasing the strain rate delays the structural transformations and, at the highest rate, changes their character toward a more abrupt and spatially dispersed response. Comparison with previous atomistic studies shows that such effects are strongly material-system dependent. A delayed onset of defect activity with increasing strain rate has also been

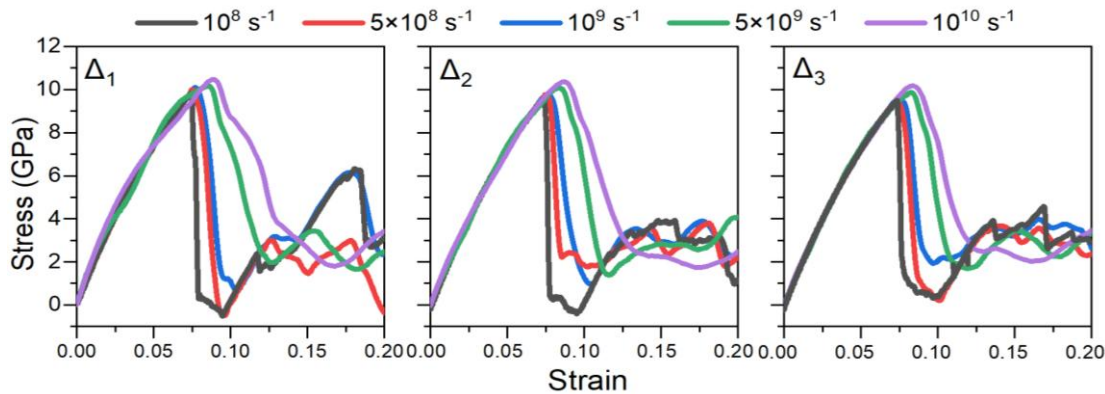


Fig. 7. Stress–strain curves of the Ni/Ti multilayers at different strain rates.

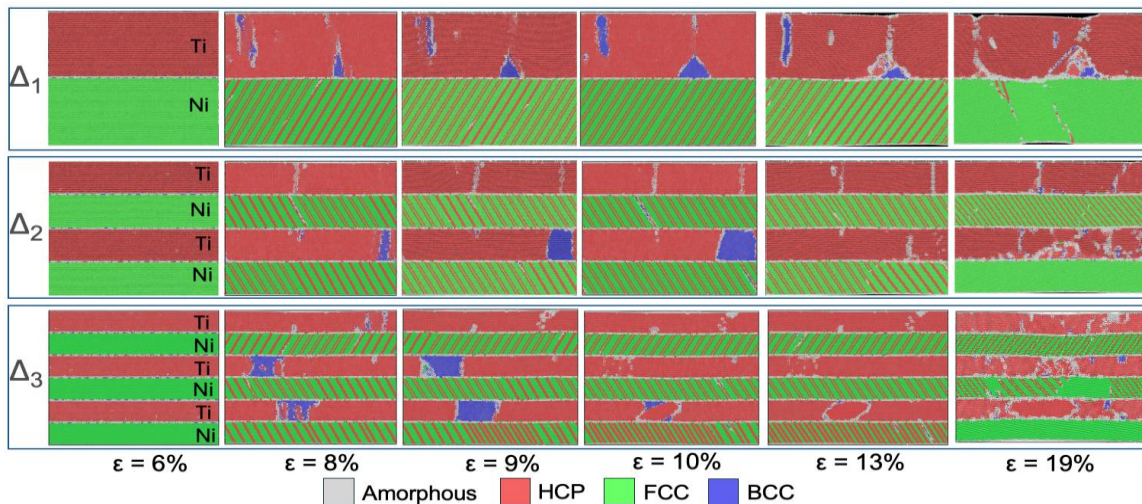


Fig. 8. Structural evolution of the Ni/Ti multilayer films with different Δ at tensile strains of 6%, 9%, 13%, and 19% at a strain rate of 10^8 s^{-1} .

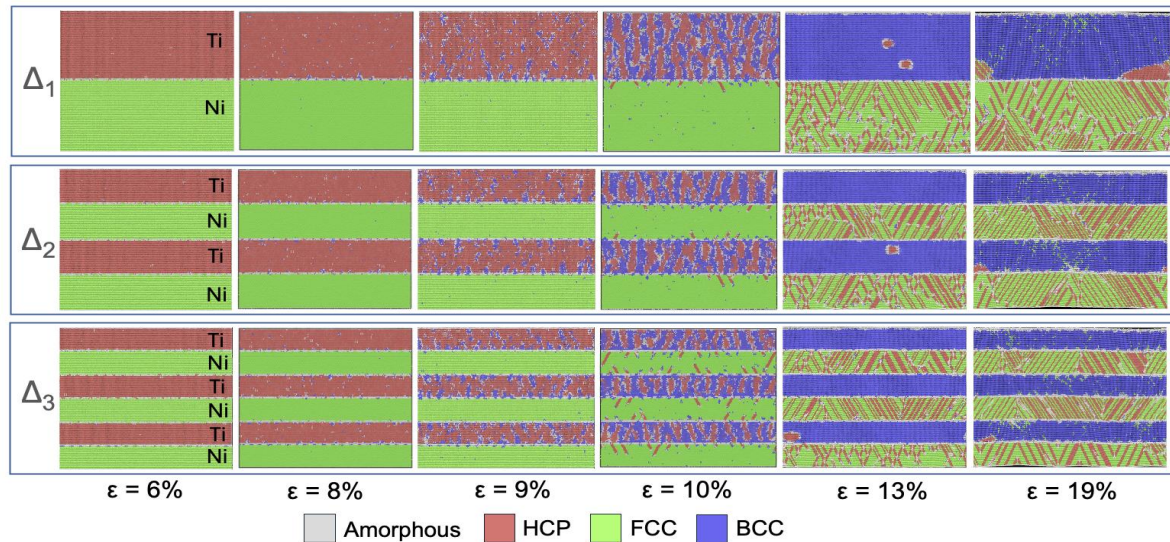


Fig. 9. Structural evolution of the Ni/Ti multilayer films with different Δ at tensile strains of 6%, 9%, 13%, and 19% at a strain rate of 10^{10} s^{-1} .

reported for Ni/Co and Cu/Ta multilayers [10-11]; however, the subsequent response ranges from substantial changes in defect evolution and deformation mechanisms [10; 15] to deformation mechanisms that remain largely unchanged over the same strain-rate range [21]. Similarly, previous studies have shown that changes in modulation period or layer thickness can substantially modify the mechanical response and deformation mechanisms of metallic multilayers [9; 11]. These differences indicate that the effects of multilayer architecture and loading rate cannot be generalized across material systems and should be established for each particular multilayer.

Conclusions

Molecular dynamics simulations revealed distinct effects of modulation period and strain rate on the tensile deformation of planar Ni/Ti multilayers. Decreasing the modulation period from 28.6 nm to 9.5 nm has little effect on Young's modulus ($140 \pm 4 \text{ GPa}$) but reduces the tensile strength from $\sim 10.28 \text{ GPa}$ to $\sim 9.49 \text{ GPa}$. Plastic deformation involves stacking-fault formation in FCC Ni and a deformation-induced HCP-to-BCC transformation in Ti. Decreasing the modulation period promotes the formation and persistence of BCC Ti and changes the partitioning of dislocation activity between the constituent

layers: Ti dominates during most of the post-yield deformation at the largest modulation period, whereas Ni carries most of the dislocation activity at the smallest period. Increasing the strain rate from 10^8 s^{-1} to 10^{10} s^{-1} produces only a moderate increase in tensile strength ($\sim 9.5 \text{ GPa}$ to $\sim 10.5 \text{ GPa}$) but systematically delays the structural transformations. Pronounced stacking faults in Ni develop at $\sim 8\%$, $\sim 9\%$, and $\sim 13\%$ strain at 10^8 s^{-1} , 10^9 s^{-1} , and 10^{10} s^{-1} , respectively. At 10^8 s^{-1} , the HCP-to-BCC transformation in Ti is also delayed and becomes more abrupt, producing finer and more dispersed BCC regions. Thus, in Ni/Ti multilayers, the modulation period primarily determines the deformation pathway and distribution of plasticity between the constituent layers, whereas the strain rate primarily controls the onset and kinetics of these deformation processes.

Acknowledgments

This work was supported by the Ministry of Education and Science of Ukraine (Project No. 0124U001266).

Palchekovskyi O. – Master student;
Orlov A. – PhD, Assoc.Prof.;
Yavorskyi Yu. – PhD, Assoc.Prof.;
Kruhlov I. – PhD, Assoc.Prof.

- [1] Y. Fu et al., *TiNi-based thin films in MEMS applications: a review*, Sensors and Actuators A: Physical, 112, 395 (2004); <https://doi.org/10.1016/j.sna.2004.02.019>.
- [2] T. Lehnert et al., *A new fabrication process for Ni–Ti shape memory thin films*, Materials Science and Engineering: A, 273, 713 (1999); [https://doi.org/10.1016/S0921-5093\(99\)00402-5](https://doi.org/10.1016/S0921-5093(99)00402-5).
- [3] H. Cho et al., *Fabrication and characterization of Ti–Ni shape memory thin film using Ti/Ni multilayer technique*, Science and Technology of Advanced Materials, 6(6), 678 (2005); <https://doi.org/10.1016/j.stam.2005.05.006>.
- [4] I. Kruhlov et al., *Structural phase transitions in Ni/Ag/Ti and Ni/Cu/Ti tri-layered thin films*, Vacuum, 233, 113999 (2025); <https://doi.org/10.1016/j.vacuum.2024.113999>.
- [5] M.A. Hollanders et al., *Amorphization along interfaces and grain boundaries in polycrystalline multilayers: an X-ray-diffraction study of Ni/Ti multilayers*, Physical Review B, 42(9), 5481 (1990); <https://doi.org/10.1103/PhysRevB.42.5481>.

- [6] O. Palchekovskyi et al., *The effect of Ni/Ti layered stack thickness on the interface amorphization behavior*, Physica Scripta, 100, 075994 (2025); <https://doi.org/10.1088/1402-4896/adeafb>.
- [7] A. Biswas et al., *Early recrystallization of Ni/Ti multilayer due to disorder in the Ni layer*, Journal of Applied Physics, 127, 165304 (2020); <https://doi.org/10.1063/5.0008177>.
- [8] S. I. Konorev et al., *Molecular Dynamics Study Of The Interface Amorphization In Ni/Ti Bi-Layered System*, 2024 IEEE 42nd International Conference on Electronics and Nanotechnology (ELNANO) (2024); <https://doi.org/10.1109/ELNANO63394.2024.10756916>.
- [9] L. Lu et al., *Molecular dynamics simulation of effects of interface imperfections and modulation periods on Cu/Ta multilayers*, Computational Materials Science, 143, 63 (2018); <https://doi.org/10.1016/j.commatsci.2017.10.034>.
- [10] A.-S. Tran, *Phase transformation and interface fracture of Cu/Ta multilayers: A molecular dynamics study*, Engineering Fracture Mechanics, 239, 107292 (2020); <https://doi.org/10.1016/j.engfracmech.2020.107292>.
- [11] T.-N. Vu et al., *Interfacial strength and deformation mechanism of Ni/Co multilayers under uniaxial tension using molecular dynamics simulation*, Materials Today Communications, 30, 103088 (2022); <https://doi.org/10.1016/j.mtcomm.2021.103088>.
- [12] L. Wan et al., *BCC stabilization and growth stress behavior in Ti/V multilayers*, Thin Solid Films, 616, 555 (2016); <https://doi.org/10.1016/j.tsf.2016.09.017>.
- [13] Z.Q. Hou et al., *Phase transformation-induced strength softening in Ti/Ta nanostructured multilayers: Coherent interface vs phase boundary*, Materials Science and Engineering: A, 684, 78 (2017); <https://doi.org/10.1016/j.msea.2016.12.040>.
- [14] H. Zhang et al., *Strain direction dependency of deformation mechanisms in an HCP-Ti crystalline by molecular dynamics simulations*, Computational Materials Science, 172, 109328 (2020); <https://doi.org/10.1016/j.commatsci.2019.109328>.
- [15] M.-J. Su et al., *Molecular dynamics study of coupled layer thickness and strain rate effect on tensile behaviors of Ti/Ni multilayered nanowires*, Chinese Physics B, 30, 096201 (2021); <https://doi.org/10.1088/1674-1056/abf10a>.
- [16] P. Hirel, *Atomsk: A tool for manipulating and converting atomic data files*, Computer Physics Communications, 197, 212 (2015); <https://doi.org/10.1016/j.cpc.2015.07.012>.
- [17] S. Plimpton, *Fast parallel algorithms for short-range molecular dynamics*, Journal of computational physics, 117(1), 1 (1995); <https://doi.org/10.1006/jcph.1995.1039>.
- [18] Y.-K. Kim et al., *Development and application of Ni-Ti and Ni-Al-Ti 2NN-MEAM interatomic potentials for Ni-base superalloys*, Computational Materials Science, 139, 225 (2017); <https://doi.org/10.1016/j.commatsci.2017.08.002>.
- [19] B. Liu et al., *Molecular dynamics simulation of the porosity effect on transformation mechanism of nanocrystalline porous NiTi shape memory alloy*, Materials Today Communications, 34, 105320 (2023); <https://doi.org/10.1016/j.mtcomm.2023.105320>.
- [20] A. Stukowski, *Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool*, Modelling and simulation in materials science and engineering, 18(1), 015012 (2010); <https://doi.org/10.1088/0965-0393/18/1/015012>.
- [21] Y. Zhang et al., *Tensile and compressive behavior of TiN/Cu layered composites: A molecular dynamics study*, Computational Materials Science, 271, 114817 (2026); <https://doi.org/10.1016/j.commatsci.2026.114817>.

О. Пальчевський¹, А. Орлов¹, Ю. Яворський¹, І. Круглов¹

Деформування розтягом багатошарових систем Ni/Ti: сукупний вплив періоду модуляції та швидкості деформації за результатами моделювання методом молекулярної динаміки

¹Національний технічний університет України «Київський політехнічний інститут імені Ігоря Сікорського», Київ, Україна, yu.yavorskyi@kpi.ua

Механічний відгук багатошарових систем Ni/Ti визначається взаємодією між деформаційними процесами, опосередкованими міжфазними межами, та структурними перетвореннями в окремих шарах. У цій роботі методом молекулярної динаміки досліджено деформацію розтягом планарних багатошарових систем Ni/Ti з періодами модуляції від 28,6 нм до 9,5 нм за швидкостей деформації від 10^8 c^{-1} до 10^{10} c^{-1} . Зменшення періоду модуляції знижує міцність при розтязі приблизно на 8% та суттєво змінює характер деформування після досягнення границі плинності, зокрема розподіл дислокаційної активності між шарами Ni і Ti, а також утворення та збереження деформаційно-індукованої ОЦК-фази Ti. Збільшення швидкості деформації має порівняно слабкий вплив на міцність при розтязі, проте систематично затримує структурні перетворення. Виражені дефекти пакування в Ni формуються за деформації ~8% при швидкості 10^8 c^{-1} , але лише за ~13 % при 10^{10} c^{-1} . За найвищої швидкості деформації перетворення ГЦП→ОЦК у Ti також затримується та відбувається більш різко, що призводить до формування дрібніших і більш дисперсно розподілених ОЦК-областей. Загалом результати показують, що період модуляції переважно визначає механізм деформування та розподіл пластичної деформації між окремими шарами, тоді як швидкість деформації переважно контролює початок і кінетику деформаційних процесів.

Ключові слова: Молекулярна динаміка, періоди модуляції, одновісний розтяг, механічні властивості, багатошарові системи Ni/Ti, густина дислокацій.