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Project Title: Investigating Deformation and Failure Mechanisms in Nanoscale Multilayer Metallic Composites

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Contents

Executive Summary

Over the history of materials science there are many examples of materials discoveries that have made superlative materials; the strongest, lightest, or toughest material is almost always a goal when we invent new materials. However, often these have been a result of enormous trial and error approaches. A new methodology, one in which researchers design, from the atoms up, new ultra-strong materials for use in energy applications, is taking hold within the science and engineering community. This project focused on one particular new classification of materials; nanolaminate metallic composites. These materials, where two metallic materials are intimately bonded and layered over and over to form sheets or coatings, have been shown over the past decade to reach strengths over 10 times that of their constituents. However, they are not yet widely used in part because while extremely strong (they don't permanently bend), they are also not particularly tough (they break relatively easily when notched).

Our program took a coupled approach to investigating new materials systems within the laminate field. We used computational materials science to explore ways to institute new deformation mechanisms that occurred when a tri-layer, rather than the more common bi-layer system was created. Our predictions suggested that copper-nickel or copper-niobium composites (two very common bi-layer systems) with layer thicknesses on the order of 20 nm and then layered 100's of times, would be less tough than a copper-nickel-niobium metallic composite of similar thicknesses. In particular, a particular mode of permanent deformation, cross-slip, could be activated only in the tri-layer system; the crystal structure of the other bi-layers would prohibit this particular mode of deformation.

We then experimentally validated this predication using a wide range of tools. We utilized a DOE user facility, the Center for Integrated Nanotechnology (CINT), to fabricate, for the first time, these tri-layer composites. CINT formed nanolaminate composites were tested in tension, with bulge testing, using nanoindentation, and using micro-compression testing to demonstrate that the tri-layer films were indeed tougher and hardened more during deformation (they got stronger as we deformed them) than equivalent bi-layers.

The seven graduate students, 4 post-docs and research faculty, and the two faculty co-PI's were able to create a collaborated computational prediction and experimental validation team to demonstrate the benefits of this class of materials to the community. The computational work crossed from atomistic to bulk simulations, and the experiments coupled form nm-scale to the mm scale; closely matching the simulations. The simulations provided viable mechanisms that explained the observed results, and new experimental results were used to push the boundaries of the simulation tools. Over the life of the 7 years of this program we proved that tri-layer nanolaminate metallic composite systems exceeded the mechanical performance of bi-layer systems if the right materials were chosen, and that the mechanism responsible for this was tied to the cross slip of dislocations. With 30 journal publications resulting from this work we have broadly disseminated this family of results to the scientific community.

1. Introduction

Nanoscale multilayer metallic (NMM) material systems, such as nanolaminate and nanowire composites when properly designed, can exhibit remarkable mechanical and electrical properties with good thermal stability and resistance to harsh environments. When designed to have high interface-to-volume ratio and chemically and topologically stable interfaces, they can posses superior strength, high resistance to fatigue damage and tolerance to irradiation damage. Understanding the physical origin of these phenomena and their relation to the interface structure, chemical composition and topology, as well as to the underlying dislocation mechanisms, is critical to designing such nanocomposites with desired properties for various applications. Thus, the main goal of this investigation was to advance the fundamental understanding of deformation, strength, damage, and failure mechanisms of NMM composites under various loading and environmental conditions with a focus on trimetallic NMM composite systems.

NMM composites are typically made of bimetallic systems with either coherent or incoherent interfaces. For example, the fcc/fcc CuNi systems with cube-on-cube orientation have a coherent interface where the atomic arrangement and slip systems are continuous across the interface, while the fcc/bcc CuNb system with the Kurdjumov-Sachs orientation has an incoherent interface where slip systems are not continuous. It is generally understood that coherent systems are more ductile and their increased strength is determined to a large extent by the ability of the interfaces to act as barriers to dislocation transmission between layers. Incoherent interfaces are generally stronger; they act as barriers to slip transmission, are weak in shear, and act as dislocations sinks, resulting in the shearing of the interface. Recent studies on CuNb revealed that incoherent interfaces can also act as sinks for radiation-induced defects, making these systems candidates for use in radiation environments.

This project studied the behavior of a new class of NMM composites of hybrid coherent/incoherent interfaces (trimetallic systems) that was based on the hypothesis that it might be possible to design a trimetallic NMM composite which might possess more superior properties than the two types of bimetallic systems discussed above. This might be achieved by building a new system that combines the two bimetallic systems with their respective interface strengthening mechanisms and properties. Towards this end, this research had the following objectives:

1. Investigate, both experimentally and through molecular dynamics (MD) and dislocation dynamics (DD) sstudies, the strength and creep-fatigue behavior of NMM composites under moderate to high temperature, strain rate.
2. Investigate the effect of interface structure, morphology and imperfections on strength and deformation mechanisms of NMM through MD studies.
3. Investigate deformation and failure mechanisms of NMM composites through DD analysis enhanced by information from MD of dislocation interaction with interface and interfaces-imperfections.
4. Establish relationships between strength, toughness, and fatigue resistance as a function of materials, interfacial properties and layer thicknesses.

2. Summary of Project Activities and Accomplishments

This research project focused on investigating a new class of materials composed of trimetallic nanoscale multilayer metallic (NMM) composites comprising hybrid coherent/incoherent interfaces. The activities involved the following:

a) Fabricate and characterize the structure of trimetallic NMM composites with minor interfacial impurities. DOE user facility, the Center for Integrated Nanotechnology (CINT), was utilized to fabricate, for the first time, tri-layer composites.
b) Perform mechanical tests, including uniaxial and biaxial bulge fatigue, creep-fatigue, and monotonic tests of trimetallic NMM composites, with and without exposure to radiation, as a function of temperature and atmosphere (oxidizing versus reducing environments).
c) Perform molecular dynamics studies of interface mechanics in trimetallic NMM to investigate possible interface imperfections and interface chemistry.
d) Perform dislocation dynamics studies of dislocation mechanisms in trimetallic NMM composites and of interface crack-dislocations interaction.

Three Postdoctoral Fellows, five PhD students, and two MS students were involved in this project, either full time of part time. The result from this work is reported in 32 journal articles [1-32]. The result from the molecular dynamics investigations are reported in [7-11, 15, 21, 23-26,30, 32], and those from dislocation dynamics studies are given in [1,2,4-,6,18,19]. Guided by these results, multilayer thin films of CuNbNi with various layer thickness where fabricated at CIN and tested at WSU in tension, with bulge testing, using nanoindentation, and using micro-compression to demonstrate that the tri-layer films were indeed tougher and hardened more during deformation (they got stronger as we deformed them) than equivalent bi-layers [3,12,16,17,22,27,29,31].

These discoveries led the research team to investigate other bilayer and trilayer material systems (MoPtNi, Ni/Np-Au and CrCu) [13], and consider developing more complex multilayer nanostructured metallic systems, NNM with nano-precipitates and into three-dimensional foams with nanolayered struts, and finally metallic-ceramic nanolaminate systems (Nb/Nbc). It was shown first numerically through MD investigations and then experimentally, that by adding nano-precipitates within the NMM system one have the opportunity to further enhance strengthening [20,27] and enlarge the design size-space. In the case of foam structures, it was shown, again first numerically then experimentally, that it is possible to increase the overall strength of nanoporous materials by forming a core-shell structure with composite ligaments [22]. Specifically, adding thin layers of Ni onto a NP-Au foam can increase the strength of the film by approximately five times in the core-shell foam [22]. The addition of Ni does not only impact the hardness, but also significantly decreases creep during the indentation process. Finally, the research team studied a metallic-ceramic nanolayer composite system Nb/Nbc [28, 30, 32]. Details of the main accomplishments are given next.

3. Detailed Summary of Accomplishments

3.1 Plastic deformation, strength and strain hardening in NMM

Biaxial testing, microtensile, nanoindentation and microcompression methodologies were developed to carry out tests at and near the plastic deformation limit to quantify the onset of plasticity, separating us from the majority of the work in the literature that examines flow stress at larger strains. Bilayers of CuNb, CuNi, CrCu, NiNp-Au as well as trilayer film composites of CuNiNb, MoPtNi were fabricated and tested. Material fabrication was carried out jointly at WSU and at the CINT facility in LANL. The mechanical properties of the films were measured using bulge testing and nanoindentation. Elastic and plastic properties were determined for freestanding films and reported in [3,12,13,16].

Bulge testing of free standing membranes was used to identify the initial yielding behavior for the multilayers during the first portion of this contract. The pressure at which yield first occurred was identified from the pressure deflection data, and using the von Mises stress at the center of the membrane, the maximum stress was determined. The highest applied stress in each membrane at the point of initial yield, as determined from this previous study, is shown for the different chemistries in Figure 1. The use of a square, rather than rectangular membranes, led to significant non-uniform deformation in the free standing films which precluded an accurate conversion to unaxial stress strain beyond the first yield point, and therefore larger strains were probed using nanoindentation.

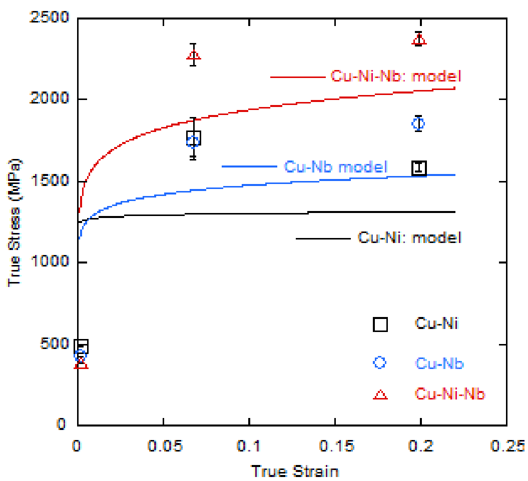


Figure 1. Effective flow stress at different strains for the three multilayered chemistries estimated using bulge testing and nanoindentation. Data points for strains of 7 and 22% are averages of 36 indentations with error bars equal to the standard deviation. Data points at 0.2% are based on yielding data from bulge testing. Fits follow eq (3) with fixed values of strain hardening exponents shown in Table 1.

Nanoindentation with a Berkovich and cube corner diamond tip was used to measure the modulus and hardness of the films at different effective strains (Figure 2). The pile up around an indent can also be related to the strain hardening behavior of a material; materials that strain harden exhibit less pile up than materials which show perfectly plastic behavior. The choice of the cube corner tip as a second probe of indentation behavior serves a dual purpose; allowing the determination of hardness at a higher effective strain than the Berkovich tip while at the same time ensuring that the pile up around the indents is large enough to be measurable and is not dominated by the surface roughness of the films.

Nanoindentation was carried out using a Hysitron Triboindenter with a partial unload technique to evaluate the properties at 15 different depths for each indentation. 36 indents were used for determining the properties of each film and indenter tip. The hardness values reported here refer to averages of values measured at contact depths that correspond to an effective contact radius of approximately 20% of the film thickness (i.e. for a Berkovich tip a depth of about 5% of the film thickness). The modulus at this depth was similar to the modulus measured via bulge testing, ensuring substrate effects were minimal. The pile up around the indents was measured by scanning the surface using the Hysitron imaging capabilities and recording the residual impression topography.

The stress and strain values determined from both nanoindentation and bulge testing are engineering values and are accordingly translated to true stresses and strains when presented in Figure 1 using the common uniaxial conversion for convenience. The multilayer that shows the highest initial yield stress (Cu-Ni) did not exhibit the highest hardness. The trilayer film has the lowest initial yield stress, but has the highest hardness with the Berkovich tip. The amount of upheaval *h* around a residual indentation can be related to the strain hardening coefficient of the material. For a given indenter, using the contact radius of the residual impression and the upheaval *h* measured from the topographical scans of the sample surface, the constant *c* can be calculated and subsequently related to the strain hardening exponent. Figure 2 shows the topography around typical cube corner indents for the Cu-Ni and the Cu-Ni-Nb films along with the corresponding height profiles; averages and standard deviations are shown in Table 1. The differences are indicative of the different strain hardening behavior for the three films. The differences in the amount of pile up were found to be statistically significant using the Wilcoxon Rank Sum test. Probability values less than a cutoff value; selected here as p=0.05, indicated the three data sets were from statistically different populations.

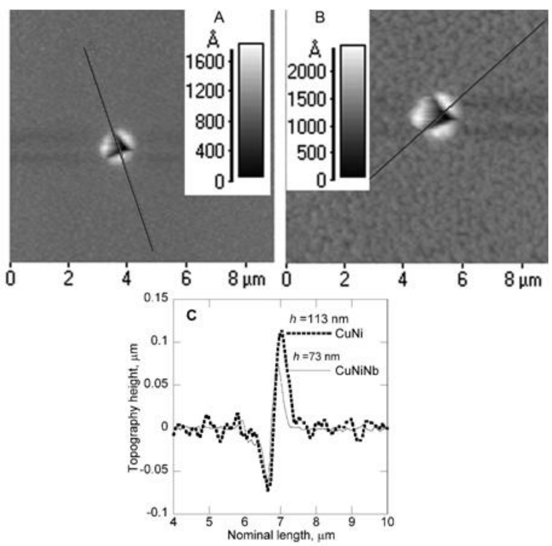


Figure 2. Topography around a cube corner indent on the (A) Cu-Ni-Nb multilayer and (B) the Cu-Ni multilayer. The corresponding height profile along the line marked in each figure is shown in (C); for the same projected contact area the pile up is substantially higher in the bi-layer film than the tri-layer film.

Table 1. Normalized pile-up ratios (*h/a)* for the three multilayers used in this study along with the strain hardening exponents calculated using the Bower model for frictionless indenters

Multilayers	*h/α*	*n*
Cu-Ni (20 nm-20 nm)	0.231$\pm$ 0.033	0.01
Cu-Nb (20 nm- 20 nm)	0.197$\pm$0.026	0.055
Cu-Ni-Nb (20 nm-20nm-20nm)	0.175$\pm$0.014	0.084

The data presented in Table 1 show that the Cu-Ni multilayers that pile up the most correspond to the lowest strain hardening exponent, while the Cu-Ni-Nb multilayers pile up the least showing the largest strain hardening. These trends agree with those shown by the combination of bulge testing and nanoindentation data where the Cu-Ni film, which has the highest initial yield stress, is not the hardest in nanoindentation, showing limited capability for strain hardening compared to the Cu-Ni-Nb trilayer which exhibits significant strain hardening. The corresponding fits for each data using a conventional power law hardening model are presented in Figure 1, and while the values do not match exactly, the trend in behavior is the same between the simple analytical model and the experiments.

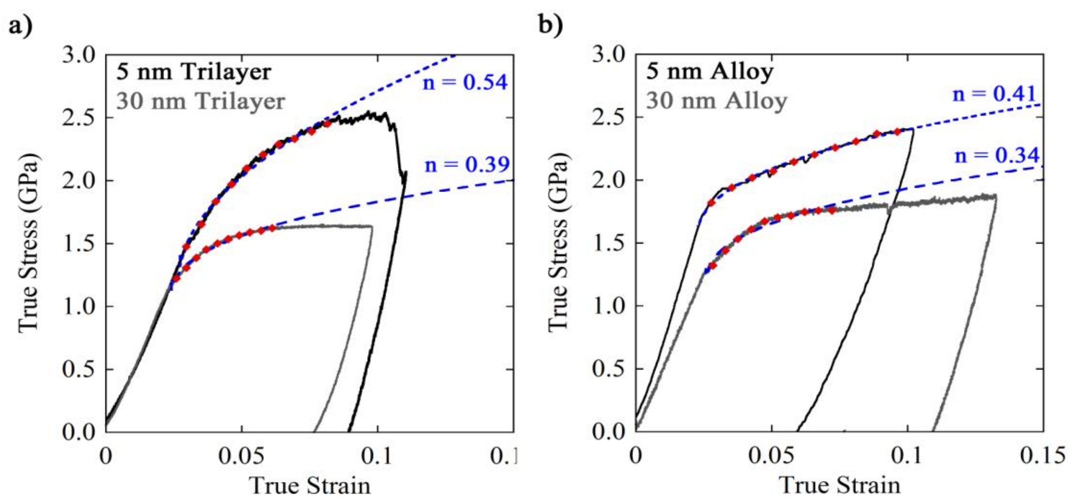


Figure 1. Example of stress-strain curves from micro-pillar compression testing of NMMs for (a) tri-layer, mixed interfaces and (b) the bilayer alloy (incoherent interface only) films.

Micropillar compression testing was also used in this investigation to allow for more accurate determination of the strain-hardening exponent of these NMMs [32]. Traditionally, these pillars are fabricated using focused-ion beam (FIB) milling which has the tendency to create pillars with a slight taper which can be accounted for by a first-order correction. Tri-component films of Cu/Ni/Nb NMM films were deposited using magnetron sputtering on (100) oriented Si starting and ending with the Nb layer to a total thickness of 3 μm with equal individual layer thicknesses of 5 and 30 nm. A second set of samples was fabricated to investigate the specific role of the FCC/FCC interface while maintaining the overall chemistry of the tri-layer; these samples began with a 5 or 30 nm Nb layer, but then used co-deposition sputtering to create a 10 or 60 nm thick FCC alloy layer. The alloy system was deposited to a total thickness of 1.6 □m, the repeating period of layers was constant between the alloy and tri-layer system. The micro-pillar compression tests were conducted in a Zeiss DSM 962 SEM with a modified Alemnis *in situ* indenter using displacement control loading and conducted at strain rates of approximately 1e-3 /s. Taper corrections were applied to the load-depth curves and resulted in the true stress-true strain curves shown in Figure 3. In this case, the substrate stiffness is sufficiently higher than the tri-layer films, so the effect of pillar sink-in into the substrate compliance was found to be negligible. The beginning of each curve is slightly non-linear due to rounding of the top of the pillar from FIB milling, therefore, the curves were offset so that the extrapolated elastic portion crosses the origin. The compression results show a clear hardening behavior in both layer thicknesses. Examination of the pillars after testing (Figure 4) shows barreling in the alloy films that is not accounted for in the first order taper correction calculations. This would lead to additional perceived hardening that is not seen in the tri-layer films. The results from these experiments can be described in light of the confined layer slip model, and supports the hypothesis that coherent interfaces with a modulus mismatch in the tri-layer system are responsible for additional deformation mechanisms that can lead to hardening in excess of that found in bi-layer systems.

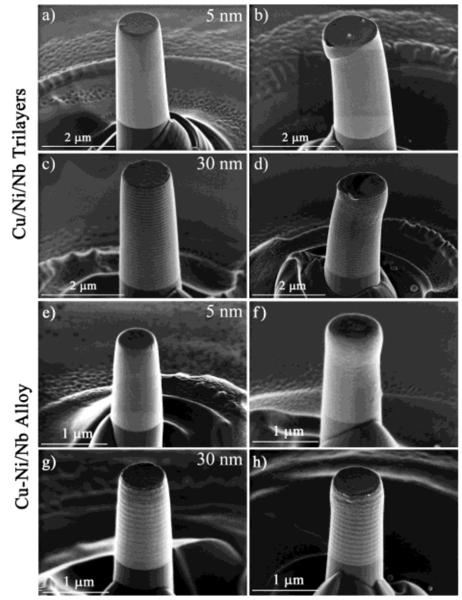


Figure 2. As deposited (left) and post mortem pillars of mixed interface tri-layer films (a-d) and incoherent interface alloy films (e-h) showing difference in deformation as a result of interface type and layer thickness.

The effect of variations in the Nb layer thickness in trilayer systems was also investigated.. Based on the MD simulations [7,14,17], Cu/Ni/Nb thickness between 5/5/4 and 5/5/1 should show properties that exceeded that of a uniform thickness . These films were fabricated at the CINT facility in LANL, etched to create free standing membranes at WSU, and tested with bulge testing nanoindentation. Figure 5 shows the representative harnesses of the trilayer films with variable Nb thickness. While the trend is similar to the MD predictions of performance, the most important aspect of this result is that the scale of the MD predictions is clearly tied to the experimentally measured hardness. The hardness of a 5/5nm Cu/Ni or a 5/5 nm Cu/Nb films from literature is shown in Figure 5 also, and true to the MD predictions (Figure 12 below) the 5/5/3 Cu/Ni/Nb films are between these values.

The initial experimental studies of yielding were designed to further develop fatigue testing procedures. Several issues aroused as a result of these studies. As the conventional method of fatigue testing is based on stress amplitudes and various ratios between yield and ultimate tensile strength, it was not clear at what point one might expect cyclic hardening or softening. Based on the work of Misra at LANL, which showed relatively low strain hardening above 20% strain there was a concern that multilayer films might cyclically soften. However, as we have now demonstrated that the initial yield behavior is actually significantly lower than the flow stress at 8% strain in these systems and that they do show significant strain hardening in the 0.01-20% range, one should expect cyclic hardening, not softening. We have begun fatigue testing on all of the systems, and to date have not been able to observed any damage accumulation in stress controlled tests at the yield strength on the order of 500 cycles. This is both a benefit (i.e. fatigue appears to be less of an issue than previously imagined) and a problem for further testing, as the pressures required for fatigue testing largely exceed those which can be applied in our current bulge testing system. Further work will be needed to either modify the testing apparatus for loading to higher base pressures or to significantly increase the rate of fatigue testing to sample statistically significant numbers of samples.

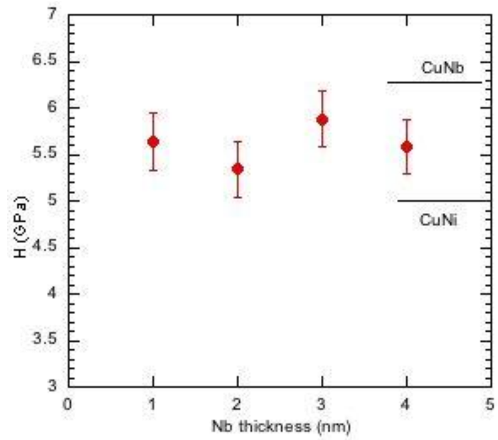


Figure 5. Indentation hardness and initial yield strength of Cu/Ni/Nb films.

Finally, as service conditions include possible thermal treatments, we initiated an ancillary project beyond the initial scope of work to assess the effects of oxidation on the properties of NMM composites. As Cu, Ni, and Nb all can oxidize, we selected Pt/Mo to examine this behavior, as Pt is resistant to oxidation and would confine oxidation to Mo. The results of this structure oxidizing were unexpected: thicker layers of Pt/Mo withstood annealing better than thinner layers because the interface structure was maintained even as the oxidation of the Mo occurred [12,3]. Figure 7 shows the growth of the oxide layer is constrained to the Mo layers. Even partial oxidation led to increases in hardness. Future studies of trilayer films proposed in the renewal proposal will need to consider the complex interactions between the constituent materials and the environment. Also of

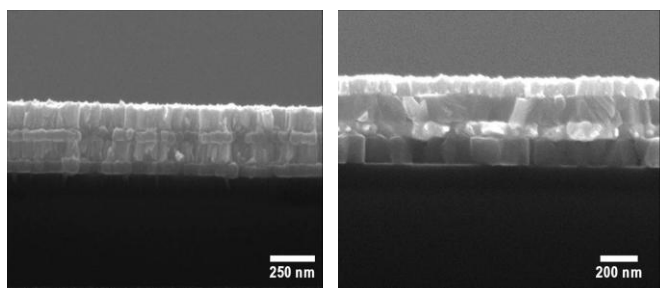


Figure 6. Pt/Mo multilayers before (left) and after (right) oxidation showing growth in the Mo layer while maintaining the layered

interest in this system was the fact that moderate amounts of hardening occurred even at room temperature as the highly stressed layers allowed oxidation of the Mo (identified using XPS). The hardness increased over the course of 3 months by up to 20%; this indicates the very real possibility that impurities could provide additional strengthening mechanisms in NMM composites, and will be considered in our future studies.

3.2 Elevated temperature dependence of hardness in NMM

The tri-layer nano-scale metallic multilayer (Cu/Ni/Nb) system with a mixture of incoherent and coherent interfaces was investigated to determine the effect of elevated temperature conditions on the strength at temperature and after annealing [29]. Elevated temperature nanoindentation showed a reduction in the temperature sensitivity of hardness as individual layer thickness decreases (i.e. thinner layers retain strength better at elevated temperatures). A summary of the experimental results for elevated temperature indentations tests into the 30 nm thick layered system is shown in Figure 7. The hardness of all three tri-layer films decreases as the temperature increases However, by comparing the relative drop in hardness, it is clear that thinner layers are more resistant to mechanical degradation than thicker layers. Across a 300 K temperature range, the hardness of the 30 nm sample drops by 35% while the 5 nm sample only drops by 15%. Since this system includes two sets of miscible systems (Cu–Ni and Ni–Nb) and may have some interface broadening, CuNi alloying and the formation of NbNi precipitates can occur. This has the potential to either weaken the system through layer degradation, or possibly add additional strengthening from dislocation interactions with the new solid solution layer or precipitates and will be the focus of future investigations.

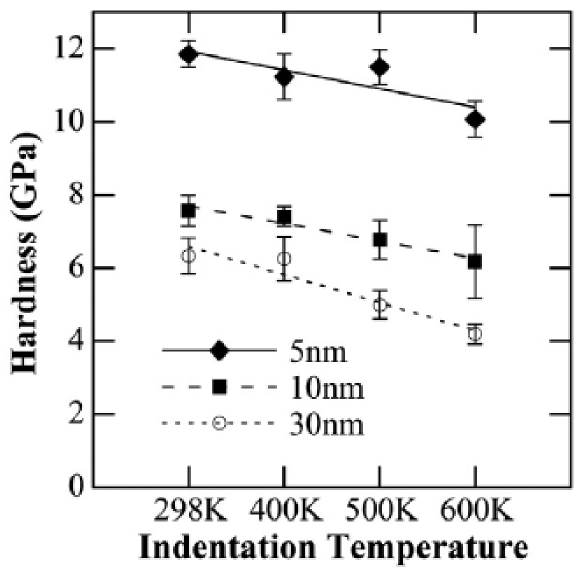


Figure 7. Summary of elevated temperature indentation for the three layer thicknesses at four different temperatures. The room temperature data is from the post-annealed condition.

MD simulations of Cu/Nb bilayers was conducted in order to examine the mechanical response of tri-layer NMMs d at elevated temperatures [25]. Typical results are shown in Figure 8. The MD results supports the experimental findings and show hardness having a decreasing temperature sensitivity as the layer thickness decreases for multilayer films within the range in which strength is dominated by the confined layer slip model. Since these layer thicknesses are all in the range in which the CLS model describes the deformation mechanism, it appears that the change in temperature sensitivity is not a result of a different dislocation process but rather the interaction of dislocations with the interface. Simulations conducted at 500 K further show that at larger layer thicknesses additional slip planes are activated, leading to the decreased strength observed in both the simulation and experimental results. Post-annealing indentation shows that the tri-layer system is resistant to significant degradation in strength when annealed to 600 K for 4 h. Additional evidence of strengthening after annealing suggests the possibility of local interfacial changes, from either small amounts of Cu/Ni intermixing at the interface or the addition of very small NbNi precipitates at the Nb/Ni interface, both of which could enhance strength in these systems.

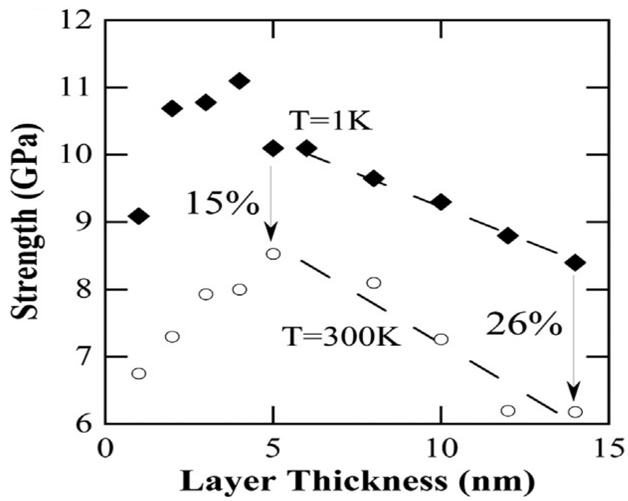


Figure 8. Summary of MD simulation results indicating the effect of temperature on the second yield point as a function of layer thickness for thicknesses ranging from 1 nm to 14 nm. Details of this simulation can be found in reference.

3.3 Precipitation Strengthening in NMM

In this part of the study we explored the possibility of increasing the strength of the NMM by adding nano-precipitates to act as obstacles of dislocation motion in the softer layer, i.e. Cu. We first carried out both MD and DD simulations [20] to investigate the interaction between a dislocation and a precipitate, followed by analytical modeling, and material fabrication and experimentation [27]. The MD results (e.g. Figure 9] suggested that a small precipitate of 1 nm radius does not affect considerably the yield stress but, as the precipitate size increases, the yield

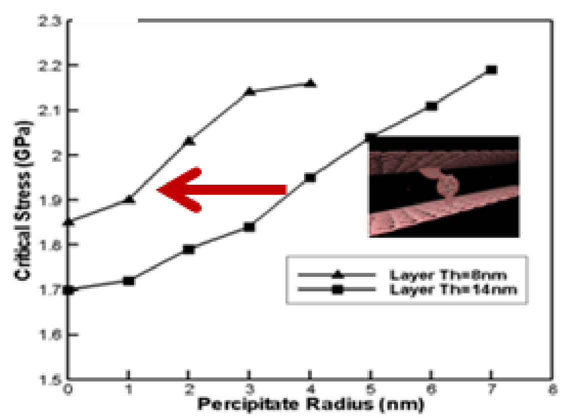


Figure 9. Critical stress as function of the precipitate size for two different structures, one with 8 nm and one with 14 nm copper layer thickness respectively. The arrow depicts the ability of the precipitates to strengthen the thicker structure to the point that it exhibits the same strength with a thinner structure without precipitates

stress increases accordingly. A larger particle would require higher additional stress in order for the dislocation to pass through. The result in Figure 5 reveals that the presence of the precipitates can lead to an increase in strength of the thicker structure. Most important, the simulations show that after a certain precipitate size the strength of the thicker structure can be made similar to that of the thinner structures without precipitates. This outcome can be used to manufacture thicker NMM's with the strength of thinner structures.

To explain this strengthening effect we developed a model based on dislocation interaction with a rigid particle in a confined channel [A19], yielding the analytical expression

$$\tau_{crit} = \frac{b\mu}{4\pi}\frac{[2-\nu(1-\cos\theta)]}{(1-\nu)}\ln\left[\frac{HD}{b^2}\left(\frac{H-D}{H+D}\right)^2\right]\frac{1}{H-D}$$

where μ is the shear modulus and ν the Poisson ratio. In the limit as $D/H \to 0$, and $D \to b$, the equation reduces to the confined layer plasticity model. The upper limit based on this equation, $D/H \to 1$, e.g. $D = H$ corresponds to the complete blockage of the channel by the precipitate and the stress becomes singular, corresponding to the breakdown of the elastic solution. However, the upper threshold is determined by the shear strength of the interface and or the precipitate as shown by the MD results. Moreover, this relation shows that both the channel width and the precipitate size control strength with inverse dependence on the mean fee path "*H-D*" and logarithmic dependence on both the channel width *H* and precipitate size *D*.

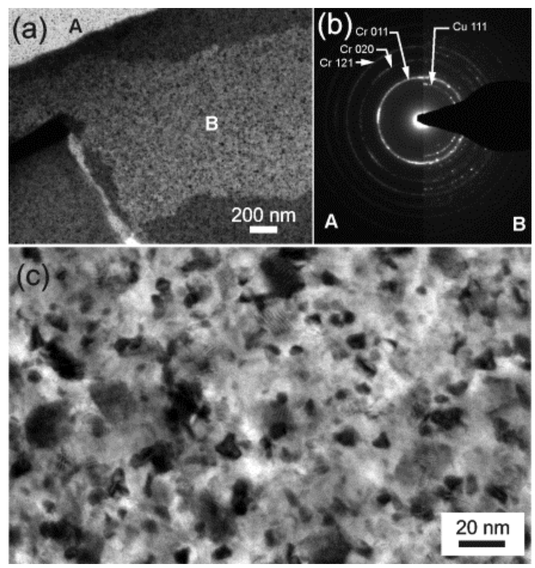


Figure 10 Bright field TEM image showing multilayer structure in a part of a 20nm as-deposited thin film. (b) SAD patterns obtained from locations indicated as A (left) and B (right). (c) Typical bright field image at higher magnifications obtained within B which includes a Cu-Cr layer.

The findings from the MD and DD simulations, and the analytical modeling, were verified experimentally by studying precipitate formation and strength in Cr/Cu-Cr multilayer films using transmission electron microscopy (TEM) and nanoindentation, respectively [27]. The Cr/Cu-Cr multilayer films were deposited using a magnetron sputtering system with a pure Cr target and a Cu-Cr (95 at.% - 95 at.%) target. Samples of bi-layer thicknesses 10 nm, 20 nm and 30 nm were deposited without specific heating or cooling. Some of these samples were annealed at100^{o}C for 30 minutes. Another set of samples were deposited at100^{o}C. A set of Cr/Cu multilayer films was also deposited for comparison.

Using the TEM, multilayer structure similar to Figure 10 (a) can be seen in all samples. Selected area diffraction patterns obtained from the Cu-Cr layers (area B in Figure A6(a)) suggest co-existence of both Cu and Cr crystals (Figure 10 (b)). Uniformly distributed particles in dark contrast within these layers (B in Figure 10 (a) and in (c)) are likely to be crystalline Cr precipitates.

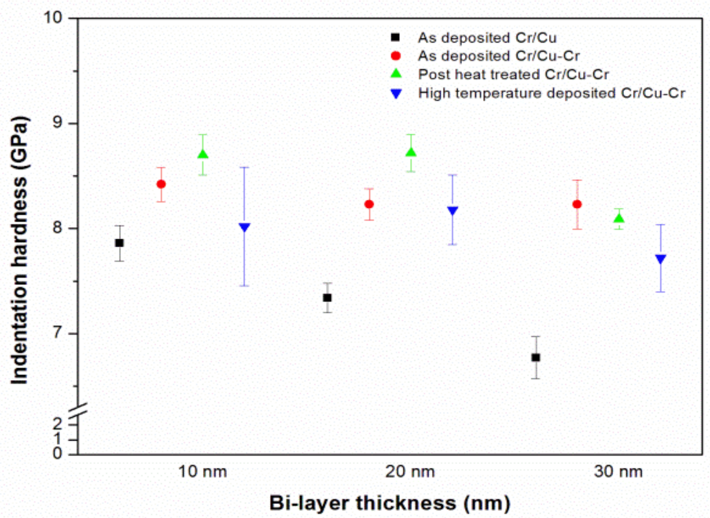


Figure 11. Nanoindentation hardness of samples deposited at four different conditions having bi-layer thickness of 10 nm, 20 nm and 30 nm. Each data point is the mean hardness of more than 80 indentations. The error bars represent the higher and lower bounds of one standard deviation from the mean.

As shown in Figure 11, hardness in these nanolaminate composites increases significantly when Cr was added to the Cu layers. More importantly, these Cr/Cu-Cr multilayer films provide strength of a 10 nm bi-layer in a 30 nm bi-layer. Higher hardness is also observed in the annealed samples. The Cr precipitates in the annealed 10 bi-layer are found to be almost 3 times larger than those in the as-deposited films. Larger precipitates are more effective in blocking dislocation, as was predicted in the simulation. In conclusion, TEM results showed that precipitates may be introduced into the Cu sublayer by sputtering with a target containing immiscible elements such as Cr. Nanoindentation results agree with the model proposed in [20] that strengthening of a nanostructured metallic material nanocomposite could be achieved through introduction of precipitates in the sublayers.

3.4 Molecular dynamics studies of mechanical behavior in NMM

Molecular dynamics studies were carried out to investigate the mechanical behavior of the NMM, with particular focus on the effect of layer thickness on the hardness of nanometallic material composites with both coherent and incoherent interfaces was investigated using nanoindentation [7,14,17,21]. The atomistic simulations were also performed to identify the critical deformation mechanisms and explain the macroscopic behavior of the materials under investigation. Nanocomposites of different individual layer thicknesses, ranging from 1–30 nm, were manufactured and tested in nanoindentation. The findings were compared to the stress–strain curves obtained by atomistic simulations. The results reveal the role of the individual layer thickness as the thicker structures exhibit somehow different behavior than the thinner ones. This difference is attributed to the motion of the dislocations inside the layers. However, in all cases the hybrid structure was the strongest, implying that a particular improvement to the mechanical properties of the coherent nanocomposites can be achieved by adding a body-centered cubic layer on top of a face-centered cubic bilayer.

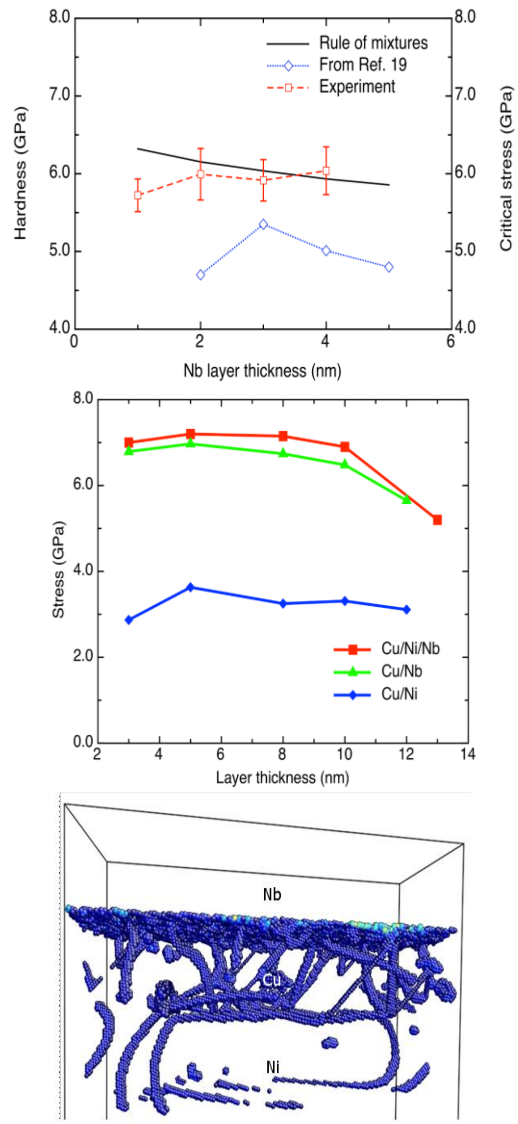


Figure 12. (top) The experimental hardness and computational shear strength of the trilayer for the case where only the Nb layer varies as a function of the Nb layer thickness. The Cu and Ni layer thicknesses are kept constant at 5 nm. (middle) The plastic stress of the Cu/Ni, Cu/Nb and Cu/Ni/Nb structures as a function of the layer thickness. (bottom) Dislocation content inside the fcc layers for the 8 nm layer thickness Cu/Ni/Nb structure. The atoms are colored according to their central symmetry parameter.

Sample results form MD simulations are shown in Figures 12a-c. The results show that the strength of the structures increases as the layer thickness decreases. The simulation results qualitatively agree with the experimental findings. Specifically, at individual layer thicknesses above 3 nm the Cu/Ni/Nb is the strongest followed closely by the Cu/Nb. In all cases, the Cu/Ni is proved to be the weakest of all. This does not change even when the structures are relaxed and loaded again with residual dislocations inside. The results reveal that the addition of Nb to Cu/Ni results to the improvement of the coherent Cu/Ni structure, increasing its strength by about 30%. However, the strength does not increase monotonically as the layer thickness decreases, because of the critical role of the interface that shears in the films with bcc layers and allows the dislocations to cross in the films with fcc layers, therefore softening the material.

3.5 Molecular dynamics studies of Strain hardening and size effects in NMM

In order to explain the strengthening effects in the trilayer system that we have observed in our experimental work [3, 13, 16,17], a series of atomistic simulations of nanoindentation were performed on several multilayer structures with different material composition, individual layer thicknesses and indenter radii and the results are reported in [23,21]. Based on the MD simulations, it was discovered that the presence of the Cu-Nb interface plays an important role on the plastic deformation of the NMM composites – it was shown its significance in both the surface pile-up deformation and the strain hardening effect of the NMM. First, for the surface deformation (pile-up and sink-in), the pile-up height is inversely related to the strain hardening rate. Two surface deformation mechanisms have been discovered, they are all affected by the presence of incoherent interfaces. Second, the hardening exponent of the NMM under nanoindentation is closely related to the shear deformation of the Cu/Ni-Nb interface. Such shear deformation, quantified by interfacial dislocation density $\bar{\rho}$, is mainly due to the dislocation-interface interactions.. The amount of the shear deformation of such incoherent interfaces, in turn, is related to the effective thickness (h^*/R) of the FCC layers, as is shown in the Figure 13. Based on these results we developed a constitutive for the hardness of the NMM composites taking the length scales, such as indenter radii and effective FCC layer thickness, as parameters, leading to the relationship:

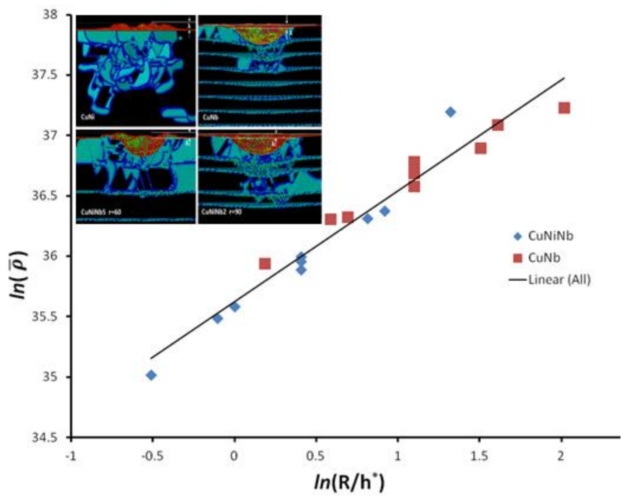


Figure 13. MD results. The dependence of interfacial dislocations and hardening on layer size and composition. Insert: Surface pile-ups and sink-ins for CuNi, CuNb and CuNiNb multilayers during nanoindentation.

$$\ln H^* = \ln H + \overline{\beta}\left(\frac{R}{h^*}\right)^m \ln(e^{\alpha}\varepsilon^{n_0}) .$$

This suggested that the hardness of a Nb, Cu and or Ni based multilayer has an inverse power law dependence on the individual layer thickness, which is qualitatively consistent with recent experimental observations [3,17]. Although this model is constructed based on a very narrow range of material combinations and individual layer thicknesses, it should apply to most of the multilayers composed of FCC and BCC material with the similar stacking setup.

3.6 Molecular dynamics studies *effect of the interface morphology*

Molecular dynamics studies were performed to investigate the effect of interfacial defect such as disconnections and interfacial dislocations on the deformation behavior. Due to discontinuity of slip systems, interfaces shear easily and act as barriers for slip transmission between layers; meaning that these interfaces have relatively low shear strengths and high potential in attracting and entrapping glide dislocations. Using MD simulations, the deformation mechanism of the interaction of the interface with upcoming glide dislocations is studied by introducing artificial dislocations inside the layer. The interface slip barrier evolves continuously during deformation by absorbing dislocations, leaving disconnections at the interface. Disconnections, which basically can be defined as the composition of a dislocation within the interface and a step, act as extra barriers for slip transmission. Quantifying the slip barriers of the interface are in strong need for analytical solutions and developing a hardening law for NMM with incoherent interfaces. From the results from the MD simulations, we developed energy maps for a sheared interface by computing the interfacial strain energy change for a various dislocation configurations and as dislocations dissolved in the interface, Figure 14a.

a) b)

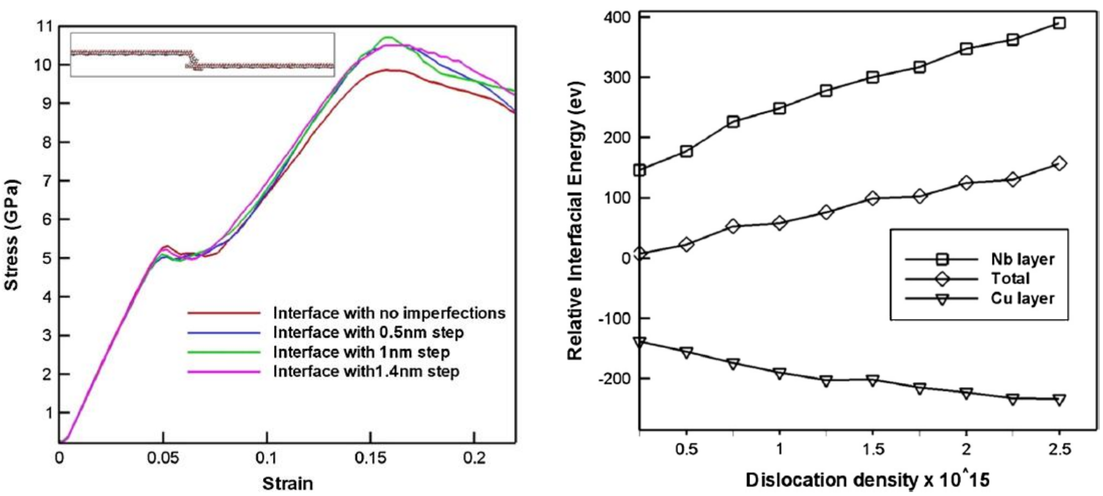


Figure 14. a) Relative interfacial energy as a function of interfacial dislocation content. b) Stress-strain behavior of a NMM with a defect free interface and other interfaces with interfacial steps of height 0.5,1.0 and 1.4 nm respectively. In the insert, an interface with a 1 nm step imperfection.

The MD results also show that disconnections can cause work hardening and increase the effect of the interface in strengthening the structure, Figure 14b. The barrier strength of the disconnection increases with increasing disconnection height. Also existence of several of these disconnections at the interface could increase this effect. These results suggests that an analytical energetic analysis able to describe the strengthening behavior of the disconnections can be based on the modification of the model developed for the case of dislocation–precipitate interaction presented elsewhere [20]. For the present problem, the layer inside which the dislocation moves will have two parts, a left part representing the initial layer thickness and a right with the disconnection that causes the reduction of the layer thickness. The thickness of the first region is represented by an initial infinite dislocation line. After a shear stress s is applied to the layer in the slip plane along the Burgers vector, the dislocation is forced to move to the second region of reduced thickness. The change of the system free energy can be then be found and the critical stress as a function of disconnection size for various layer thicknesses inside a copper layer can be evaluated similarly to the method described in [20]. In principle, the effect of a disconnection is to increase the critical stress required to propagate a dislocation inside the copper layer by reducing the thickness of the layer, and this model should reflect this fact. Overall, these studies are fundamental in the understanding of the softening behavior of NMM's and can result in designing better structures with desired properties for various applications.

3.7 Molecular dynamics studies of strain rate effects in NMM

As shown by nanoindentation, tensile/bulge, and compression experiments, the nanoscale metallic multilayers (NMM) have high strength leve under lower strain rate loading, An important aspect of the future engineering applications for such type of materials is in the field aerospace industry, e.g. the coatings on gears and bearings in aircraft engines as well as on cutting tips of the machine tools. In such cases the loading strain rates are often very high. Due to the dynamic and even destructive nature of the high strain rate loading conditions, materials' response in this circumstance often needs to be carefully addressed. Shock loading is commonly employed to study the materials' response under high strain rate loading. The failure in ductile metals is

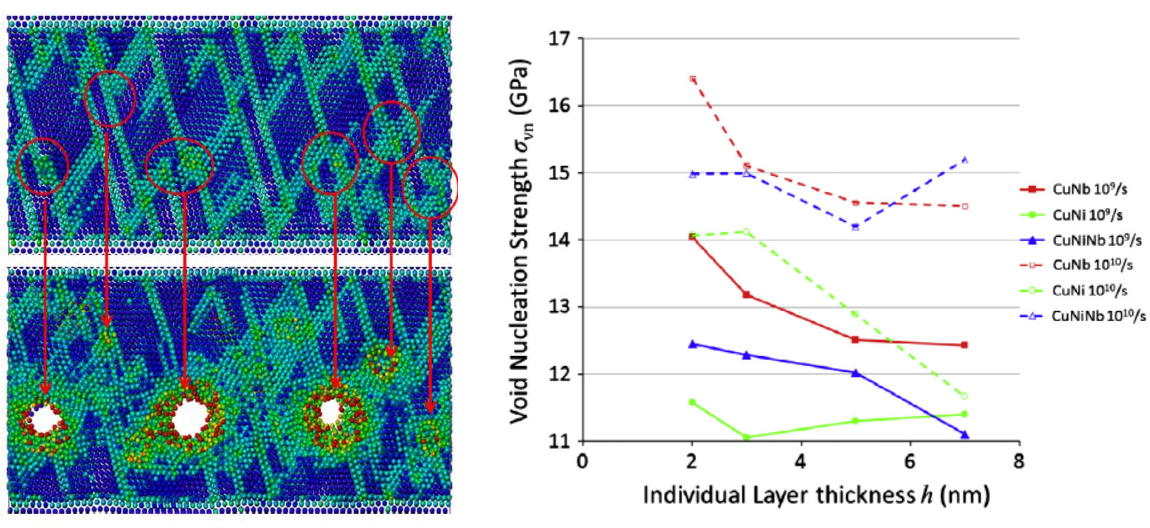


Figure 15. a) Typical void nucleation process, using Cu-Nb h= 7 nm NMM under a strain rate of 10^{10} /s as an example, the two snapshots are taken right before and after the nucleation. The nucleation sites for voids are created due to the interaction between two partials or between a partial and a stacking faculty. b) The variation of void nucleation strength with respect to the layer thickness at different strain rates.

usually related to the formation and coalescence of voids and micro cracks. In the context of shock loading, this process is often referred to as ‘‘spallation’’.

Molecular dynamics studies were performed to investigate the mechanical behavior of Cu–Ni–Nb- based nanoscale metallic multilayers (NMM) under high strain rate loadings. The simulations of NMMs with various individual layer thicknesses under uniaxial tensile strains at two different controlled strain rates (109/s and 1010/s) are performed (Figure 15b). This type of loading condition generates a stress state necessary for void nucleation commonly observed under shock loading. The mechanisms for void nucleation in the NMMs were examined and identified (Figure 15a); the void nucleation strengths (VNS) of the NMMs and their variations with respect to increasing individual layer thickness as well as available nucleation sites (affected by addition of interfacial disconnections) were obtained and explained. It was discovered that the void always nucleate from within the Cu layers, where the partial dislocations intersect with each other or with existing stacking faults. The void nucleation strength of the NMMs can be closely related to the density of available sites for void nucleation. By introducing interfacial steps into the incoherent interfaces of the NMMs the abundance of dislocation sources is changed, thus more (less) sites for void nucleation are produced which decrease (increase) the void nucleation strength of the NMMs.

3.8 Dislocation dynamics studies of mechanical behavior of NMM

Large scale dislocation dynamics studies were performed to explain the origin of the strength size effects captured experimentally, to investigate the origin of fatigue behavior by studying the interaction between cracks and dislocation, and to discover new strengthening mechanisms which are unique to trilayer systems [3, 6. 18]. We also studied the effect of Nb thickness on the load carrying capacity of the NMM composite. Some results are discussed below.

Dislocation dynamics of crack-dislocation interaction and fatigue in NMM: In order to investigate the deformation of NMM under fatigue loading condition in the presence of cracks, a numerical method was developed and integrated with the dislocation dynamics framework, to study three-dimensional cracks of any shape near an interface. The cracks are represented as distributions of infinitesimal dislocation loops [6]. The simulation provides an insight on the three-dimensional character

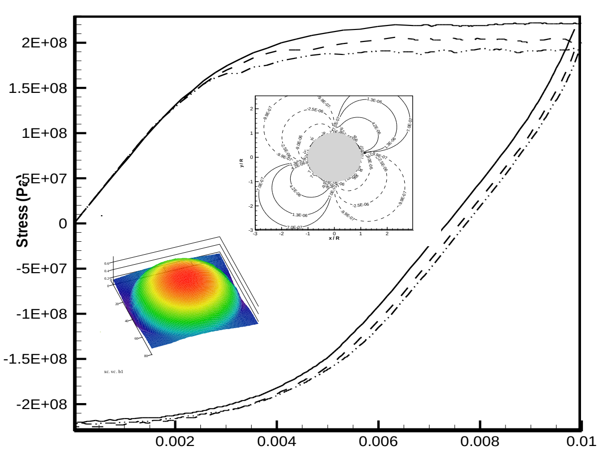
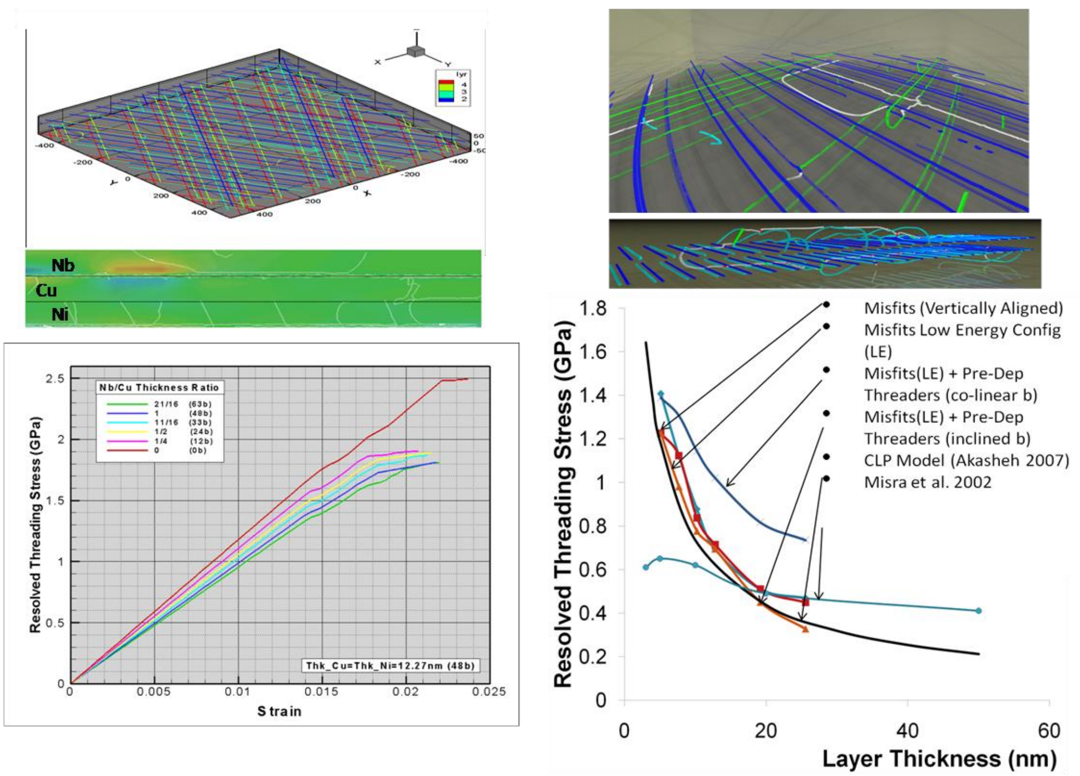


Figure 16. Fatigue plots of specimens containing a penny-shape crack. Bottom: crack opening displacement of a penny-shape crack inside the Cu layer. Top: stress distribution around the penny-shape crack.

of the dislocation structure around the cracks and its relation to the crack shapes. The effect of the cracks on the macroscopic yield stress is also determined for various crack sizes and shapes. Numerical fatigue simulations on a crystal containing nano-cracks of different shapes and sizes (Figure 16) show the presence of a nano-crack decreases the yield stress and the dislocations shield the cracks along some directions due to the configuration symmetry. However, this method is presently limited to semi-infinite films and further work is required in order to apply to NMM composites. In the renewal application, we plan to fully develop this method to include the effect of the interfaces between all layers, as explained in the methodology proposed therein. This technique will be proven very useful in the study of the fatigue behavior of NMM and will tie well with the experimental methods.



(a) (b)

Figure 17. MDDP results. a) The stress-strain behavior of a trilayer CuNiNb system with varying Nb thickness; with shearable CuNb and NiNb interfaces; the contour plot at the top of Figure 1a shows the stress distribution within the layers and the underplaying dislocation structures. b) The dependence of flow stress on layer thickness and the type of interfacial-dislocations. The figures at the top show typical dislocation structures obtained through dislocation dynamics studies.

Dislocation dynamics of mechanical behavior in NMM: The dislocation dynamics studies included a model for the coherent interface and was able to capture and explain both: a) the increase strength on layer thickness as the layer thickness decreases from 100 nm to 3 nm, and b) the drop in strength as the layer thickness is decreased below 3 nm, Figure 17 [18]. Moreover, it was possible to identify the mechanisms that contribute to hardening and that include, dislocation blocking, intersections and junctions; and dislocation mechanisms that contribute to softening and that includes dislocation crossing the Cu-Ni interface leading to the formation of “super threaders”, and dislocation cross-slip at the Cu-Ni interface as a result of the shearing of the Cu-Nb interface. This last mechanism is very interesting. It occurs even though the macroscopic state of stress (biaxial stretching) does not induce shear stress at the interface. Instead, an internal shear stress is induced as a result of the shearing of the Cu-Nb interface. This effect becomes large enough to cause cross-slip when the Cu-Ni and Cu-Nb interfaces are close, observed for thickness less than 5 nm [18].

3.9 Multiscale modeling of deformation in NMM

Based on the MD results (Figure 18), we developed a viscoplastic model to describe the deformation behavior of NMMs at continuum levels and over a wide range of layer [25]. First, using molecular dynamics simulations, we investigated the dislocation relaxation mechanisms in defining the governing plastic deformation of Nanoscale Metallic Materials (NMMs) at smaller length scales. Building on the fundamental physics of deformation as revealed from these simulations, we developed models that explain the dependence of strength on layer thickness and identify the regions where the deformation is controlled by either dislocation propagation or dislocation nucleation mechanisms. We specifically developed a molecular dynamics-based rate sensitive dislocation-nucleation-controlled model for viscoplastic flow in NMMs. The results of the simulations show that there is a transition in the operative deformation mechanism in NMMs from Hall-Petch relation to confined layer slip to interface mediated plasticity mechanisms as the layer thickness is reduced to few nm. Interface slip barrier strength decreases with decreasing layer thickness to the scale of the dislocation core leading to dislocation-nucleation-controlled deformation and thus softening of the NMMs. Based on these results, we developed a viscoplastic model to describe the deformation behavior of NMMs over a wide range of layer thickness, with the general flow rule:

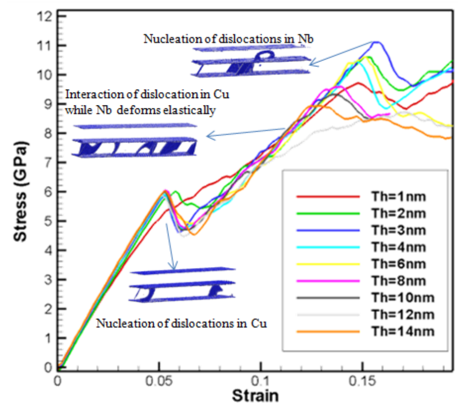


Figure 18. Stress-strain curves of the Cu-Nb NMMs under uniaxial tensile loading and with different layer thicknesses.

$$\dot{\varepsilon}_{ij}^{p} = \frac{3}{2}\frac{\dot{\bar{\varepsilon}}^{p}}{\bar{\sigma}}\frac{\partial\phi}{\partial \boldsymbol{S}_{ij}}$$

where $\dot{\varepsilon}_{ij}^{p}$ is defined according to different deformation mechanisms at different length scales as: $\dot{\bar{\varepsilon}}^{p} = \dot{\varepsilon}_0\left(\frac{\bar{\sigma}}{\sigma}\right)^{1/m}$ where

$$\begin{cases} \sigma^* = \sigma_0 + kh^{\frac{-1}{2}} & \text{for Hall-Petch region} \\ \sigma^* = M\dfrac{\mu b}{8\pi\pi}\left(\dfrac{4-\upsilon}{1-\upsilon}\right)\left[ln\dfrac{\alpha h}{b}\right]-\dfrac{f}{h}+\dfrac{C}{\lambda} & \text{for CLS region} \end{cases}$$

For small layer thicknesses where there exist no or very few initial dislocations in the layers, our simulations showed that, dislocation-nucleation mechanisms are governing the deformation behavior of the NMMs. Hence, at lower length scales:

$$\dot{\bar{\varepsilon}}^{p} = \varepsilon \upsilon = \varepsilon N \upsilon_D exp(\frac{-Q(\bar{\sigma},T)}{k_B T}) = \alpha\beta \frac{l}{h} \upsilon_D exp(\frac{-Q(\bar{\sigma},T)}{k_B T})$$

where υ_D is the rate of the nucleation of dislocations. Furthermore, using the results from numerous MD simulations, we also constructed the flow potential $\phi = \phi(S_{ij})$ via biaxial stretching of the multilayers, Figure 19. The results show that the plastic flow potential for this system is highly anisotropic and is well fitted to the Montheilet yield criteria for anisotropic materials in a first attempt. The activation parameters that are key signature for deformation mechanisms at different length scales are calculated and are on the order of those for nucleation from surfaces in nanopillars and single crystal Cu. This suggests that the calculated activation parameters are approximated reasonably within a valid range for small volume materials and are consistent with the proposed deformation mechanisms and models.

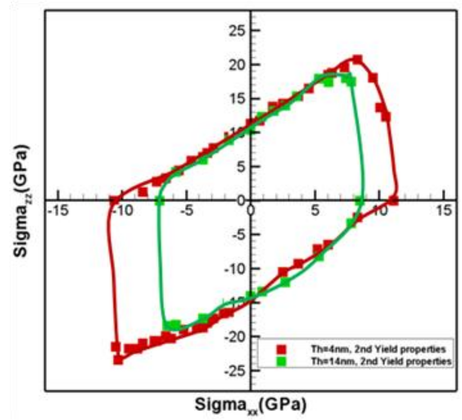


Figure 19.Comparison of yield properties for thin films with layer thicknesses of 4 nm and 14nm.

3.10 The mechanical behavior of nanoporous NMM

The results from this investigation have clearly that multilayer metallic materials have strengths in excess of either bulk constituent. Additionally, in some cases, the ability to strain harden can be enhanced due to the complex interactions that dislocations have with interfaces at small length scales. Furthermore, the confined layer slip model suggests that in some cases having layer thicknesses on the order of 20 nm will lead to dislocation motion being constrained to individual layers, due to the dissimilar elastic properties of the layers, rather than allowing dislocations to propagate across interfaces. Moreover, in certain structures such as Cu-Ni, a nanowire consisting of a copper core with a Ni shell can exhibit pseudoelasticity at large strains due to twinning [8,14,15]. Therefore, it may be possible to increase strength or relative ductility in nanoporous materials by synthesizing ligaments that consist of a core-shell structure of a nanolayered metal; this composite foam, if it behaves like a metallic multilayer, should exhibit more strain hardening capacity than the single material system [15]. In addition, if layer thicknesses were small enough, the ligaments could develop pseudoelastic properties. The added benefit of the addition of a second metal in a core-shell foam would be the addition of a broader range of elements which could be formed in the nanoporous structure. As de-alloying typically limits the system to the more noble metal, the addition of a less noble and more reactive metal may provide additional design outlets not possible from the conventional processing for these materials, as has recently been demonstrated for battery materials using tin over NP-copper.

To validate the ability to simulation and experimental data a series of Ni plated nanoporous gold films were fabricated by electrodeposition. Au ligaments were on the order of 40 nm in diameter, and Ni layers of nominal thicknesses of 2.5, 5, 8, 15, and 25 nm were deposited. The initial foam structure had a relative density of approximately 30%. Nanoindentation of both all samples were carried out, and the hardness of the resulting structures is noted in Figure 20. The values shown are averages of over 50 indentations at 4 different depths in each film to depths where the contact radius of the tip is between 0.4 and 1.0 times the film thickness.

Molecular dynamics (MD) simulations were performed using LAMMPS with potentials based on the embedded atom method (EAM) for gold and nickel. While it is possible to directly simulate a nanofoam structure within a limited volume, cylindrical ligaments with Au as the core and Ni as the shell were simulated to increase the efficiency of the calculations. The atomistic simulations show that the imitation of plasticity via nucleation of the dislocations from the Au-Ni interface and the propagation of dislocations to both core and shell layers, Figure 21. The resulting hardness from the measurements and predictions for films with nominal plating thicknesses between 0 and 15 nm are shown in Figure 19, assuming the ligament size is on the order of 35 nm and the cell size is on the order of 90 nm (i.e. a relative density of the pure NP-Au of 33%). In general, the agreement between the MD predictions and experimental

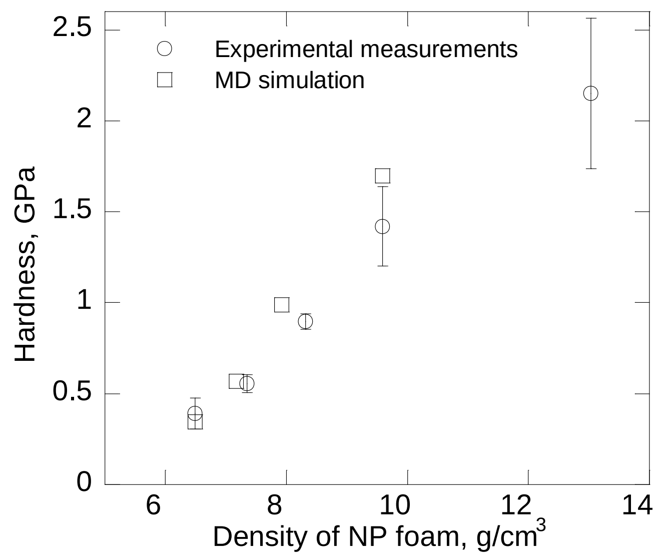


Figure 20. Hardness as a function of film density for nominal plating thicknesses of 2.5, 5, 8, and 15 nm. The experiments with plating thickness of 25 nm, which may close off regions of porosity are not included in this figure

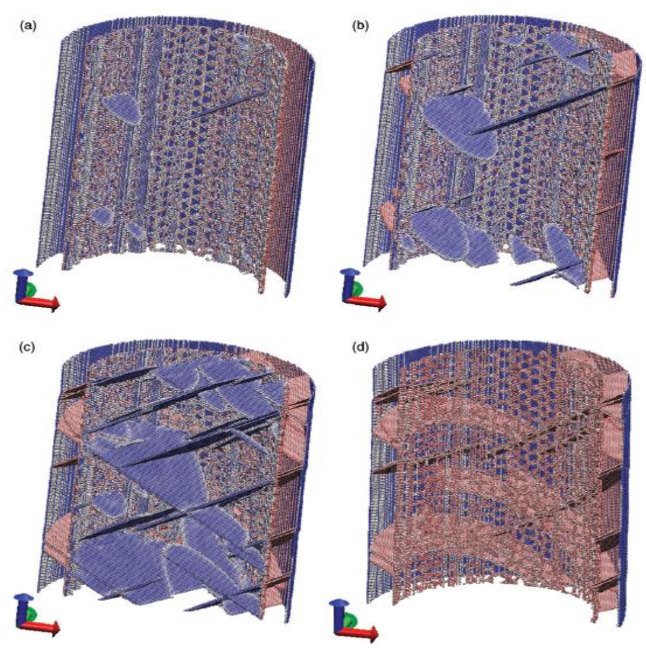


Figure 21. a) Numcleation of dislocations form the interface of Au-Ni composite legaments, b) and c) nucleation and propagation of dislocations in both Au and Ni layers, d) juts Ni layer shown at the same strain as c).

measurements is good, and lends credence to the observations in the simulations that the deformation mechanisms in a core-shell nanoporous foam differ from monolithic NP-Au.

3.11 Molecular dynamics studies of deformation mechanisms in nanoscale metal/ceramic multilayers (NMCM)

Recent advances in energy and defense-related technologies and aerospace engineering entail developing a new class of materials that can efficiently perform without premature failure under extreme loading and harsh environmental conditions. These materials are engineered to compensate for the deteriorating effect of structural and chemical defects that are inevitable in materials. In recent years, metal/ceramic multilayers have come into greater focus due to their promising mechanical, physical, and chemical properties, making them practically useful for harsh environments and extreme loading. These composites show improvement in hardness, toughness, wear resistance, thermal resistance, shock resistance, and irradiation resistance, to name a few. We have summarized the recent studies of metal/ceramic multilayers with focus on plastic deformation from three aspects: experiment, theory, and modeling. Scrutinizing the available data in the literature, we also have suggested several future research topics on the mechanical properties of metal/ceramic multilayers.

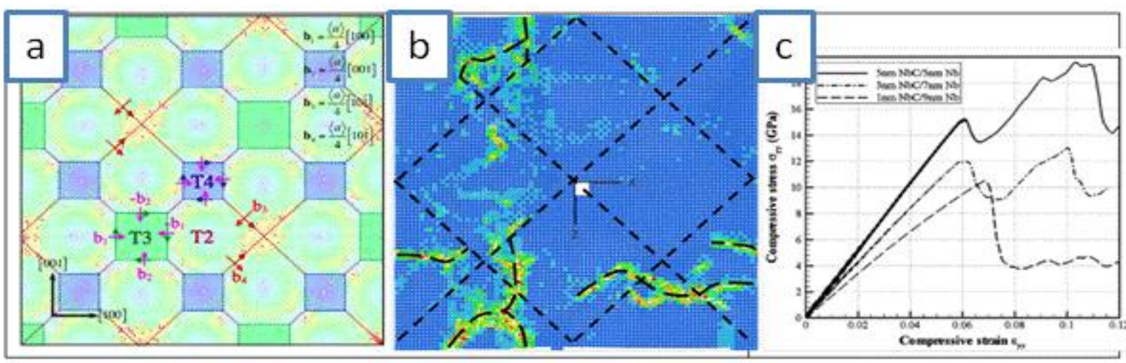


Fig. 22 (a) The plot of the disregistry analysis of the relaxed NbC–Nb interface. The dislocation lines and their Burgers vectors have been identified and marked. The plot is colored according to the disregistry magnitude. (b) Top view of atoms in the interfacial atomic layer of NbC in 1 nm NbC/9 nm Nb multilayer. Interfacial cracks are indicated as dashed lines. (c) Compressive stress–strain curves of NbC/Nb samples with 10 nm bi-layer thickness and different individual layer thicknesses.

Using molecular dynamics simulations we have studied the deformation mechanisms in Nb/NbC (metal/ceramic) multilayers and the role of interface structure and layer thickness on their mechanical behavior. The interface dislocation structure was characterized by combining MD simulations and atomically informed Frank–Bilby theory (Figure 22a). Several coherent regions exist in the interface and those are separated by misfit dislocations. MD simulations revealed node structures at the intersection of misfit dislocations. MD observations showed that plastic deformation in NbC/Nb multilayers commences first in the metal layers by nucleation and glide of lattice dislocations initiating from interface misfit dislocations. These dislocations glide in the Nb layer and are deposited at the interface. The deposited dislocations facilitate slip transmission from the Nb layer to the NbC layer in the form of several cracks. The strain hardening and the peak flow strength of NbC/Nb multilayers are associated with the slip transmission from Nb to NbC (Figure 22b), and are correlated to the interfacial dislocations, Nb layer thickness, and NbC layer thickness. The flow strength decreases with increasing Nb layer thickness and decreasing the NbC layer thickness (Figure 21c).

4. Concluding Remarks

The results from this investigation support the hypothesis that NMM composites with complex architecture can be designed which might possess properties exceeding those of the bimetallic systems. The results suggested that copper-nickel or copper-niobium composites (two very common bi-layer systems) with layer thicknesses on the order of 20 nm and then layered 100's of times, would be less tough than a copper-nickel-niobium metallic composite of similar thicknesses. Although this investigation has resulted in a considerable understanding of some of the deformation phenomena encountered in NMM composites, there remains a major gap in the understanding of the physical origin and underlying mechanism that control these phenomena, as well as a dearth of predictive models. There are numerous possibilities of NMM systems and the design space can be limitless if not guided by fundamental studies. Future research in this area should address fundamental question aiming at narrowing the design space: 1) How do interface structure, topology and imperfections affect NMM properties, and how do impurities at the interface and inside the layers impact properties? 2) What fundamental mechanisms control deformation and failure behavior in nanolaminate composites, and how is that related to the type of interface, layer thickness and precipitates? 3) What physical parameters/measures can best guide the design of nanolaminate composites (composition, interface topology, and layering scheme) for specific applications? 4) Can these concepts be extended to design a new type of three-dimensional nanolaminate-based or core-shell material systems with complex architectures and morphologies to successfully address complex loading conditions? Moreover, nanolaminate composites may improve the service life and reliability of mechanical parts in harsh energy environments, which raises the following questions: 1) How do environmental conditions (e.g. high temperature, H, He) impact the interface structure properties and the overall behavior of NMM composites? 2) How do operating conditions (pressure and strain rates) alter the behavior of NMM composites? Addressing these questions would also help guide the development of a new type of metal/ceramic nanocomposites with engineered nanolaminate structures that will exhibit higher strength, self-healing, high temperature tolerance, and thermal stability under harsh environments which has not been attempted.

5. Graduate students and Post Doctoral fellows who worked on the project

Post Doctoral Fellows and research faculty
Dr. Ioannis Mastorakos. He worked on molecular dynamics investigation of interface energy and dislocation-interface interaction; and dislocation dynamics investigations to investigate dislocation-crack interaction under fatigue. He is currently Assistant Professor at Clarkson University, NY.

Dr. Iman Salehinia. He worked on molecular dynamics investigation of interfaces. He is currently Clinical Assistant Professor at WSU

Dr. Firas Akasheh. He worked on the development of dislocation models for heterogeneous and anisotropic media. He is currently Associate Professor at Tuskegee University

Dr. Amy Wo, research faculty. She worked on material fabrication, characterization and testing. She is currently Clinical Assistant Professor at WSU. ,

Graduate Students
Dr. Rachel Schoeppner. She was a PhD student and graduated in fall 2014. She worked on mechanical testing of multilayer composite using microtensile testing methods and is currently pursing a post doc in Switzerland.

Dr. Niaz Abdolrahim. She was a PhD student and graduated in 2013. She worked on molecular dynamics investigations of interface energy and dislocation-interface interaction. She is currently a postdoctoral fellow at MIT.

Dr. S. Shao. He was a PhD student and graduated in 2013. He worked on molecular dynamics to investigate dislocation nucleation during nanoindentation of multilayered metallic composites. He is currently a postdoctoral fellow at LANL.

Dr. Aikaterini Bellou. She was a PhD student and graduated in 2009. She worked on experimental testing of strength, hardness, and fatigue, and is currently an instructor at Clarkson University.

Dr. Sreekanth Akarapu. He was a PhD student and graduated in 2009. He worked on dislocation interaction with interfaces. He is currently a Research Scientist MEMC Electronic Materials

Cory Overman. He was MS graduate student and graduated in 2009. He worked on dislocation dynamics investigations. He is currently working at PNNL.

Nicole Overman. She was a MS graduate student and graduated in 2009. She worked on mechanical testing of multilayer composite using biaxial testing methods. She is currently working at PNNL.

6. List of publications in which DOE support is acknowledged

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