Interface Structure and the Inception of Plasticity in Nb/NbC Nanolayered Composites

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Abstract

Molecular dynamics (MD) simulations were performed to explore the effect of interface structure on the inception of plastic deformation in Nb/NbC nanolayered composites. Using atomistically-informed Frank-Bilby (AIFB) method and the disregistry analysis, we characterized the structure of Nb/NbC interface, including misfit dislocations, dislocation nodes and three coherent interface structures. According to the crystallographic analysis of the interface, four possible coherent interface structures were identified. However, study of the interface energy showed that only three of them are energetically stable. After the relaxation of the interface, the unstable coherent region, which features Nb atoms in the Nb layer on the top of the Nb atoms in the NbC layer, evolves into a condensed interface dislocation node. Three stable coherent interface regions are retained in association with the formation, glide, and reaction of interface misfit dislocation loops. Disregistry analysis of the Nb/NbC interface revealed that (a) all misfit dislocations are edge type, (b) misfit dislocations enclosing the coherent extended nodes have Burgers vectors along $\langle 110 \rangle_{\text{Nb}}$. The role of the interface structure in the plastic deformation of Nb/NbC nanolayered composites was studied under two loading conditions, i.e. uniform compression and nanoindentation. Under uniform compression, lattice dislocations

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primarily nucleate from the condensed nodal regions where the local strains are the highest. Dislocations propagate in two $\{110\}$ slip planes with the same Schmid factors. Under nanoindentation, by proper positioning of the indenter, lattice dislocations nucleate from the segments of the misfit dislocations and propagate in $\{112\}$ slip planes. MD simulations also show cross-slip of lattice dislocations from $\{112\}$ planes into $\{110\}$ planes and the formation of vacancies as a result of climb of dislocation jogs.

Keyword: multilayer; interface structure; dislocation; atomistic simulation; nanoindentation

1. Introduction

Extreme loading and environmental conditions necessitate design and development of materials that show high strength and measurable ductility. These materials are also designed to compensate for the deteriorating effect of ample structural and chemical defects. In recent years, *metal/ceramic multilayers* (MCMs) have come into greater focus due to their promising mechanical, physical and chemical properties, making them practically useful in a wide range of temperatures, mechanical loadings, and environmental conditions [1]. The improvement in mechanical and physical properties of multilayers has been repeatedly linked to the thermodynamic and mechanical properties of interfaces [2–5]. The role of the interface on the plastic deformation of multilayers is multifold. Interfaces can act as barriers impeding dislocations and thus strengthening materials. The interaction between lattice dislocations and accumulated dislocations at interfaces impedes the movement of gliding dislocations in layers, causing strain hardening [4,6–14]. In addition, interfaces with high diffusivity and low formation energy for point defects can act as sinks for recovery and/or reassembly of defects to reduce stress concentrations, leading to high plastic flow stability in multilayers [15–24]. On the other hand, when the stress required to move a threading dislocation is larger than the critical resolved

shear stress for nucleating lattice dislocations from interfaces in the material, mechanical behavior of multilayered composites is mainly controlled by the nucleation and the emission of lattice dislocations from the interfaces [6,13].

Experimental [25–40], theoretical [6,29,41–44] and atomistic simulation [13] methods have been used to characterize post-nucleation of dislocations and strain hardening in metal/ceramic multilayers. Different metal/ceramic compounds have been explored under various loading conditions such as compression [25,39], tension [40], and nanoindentation [32–38]. Deformation modes such as dislocation transmission across interfaces, localized shear deformation and crack formation in metal/ceramic multilayers have been observed experimentally and studied by theoretical models and atomistic modeling [6,13,25,45]. Compared to metals, ceramics have poor plasticity at room-temperature and low fracture toughness, because of a high lattice friction stress on most slip systems at low homologous temperatures. Most of these studies show that the metallic layer undergoes plastic deformation while the ceramic layer remains in the elastic regime until it fractures. However, as the bilayer thickness is reduced to a few nanometers, compressive stress-strain curves obtained from micro-pillar compression showed that plastic co-deformability is possible in metal/ceramic multilayers [6,25]. For multilayers with the layer thickness of a few nanometers, plastic deformation is carried out by the nucleation and emission of lattice dislocations from the interfaces. Understanding the correlation between dislocation nucleation and interface structure is essential for designing metal-ceramic multilayers that have high strength and measurable formability. In situ indentation in a transmission electron microscope at a high-resolution setup has indicated the dislocation activity in both metal and ceramic layers in Al/TiN multilayers [45]. Atomic-scale modeling can reveal unit processes (involving single or a few defects) occurring at the interfaces

during deformation [46–48]. Such atomic-level findings have been partially transferred into microscale, mesoscale, and continuum-scale models to incorporate interface deformation physics [49].

The dominant effect of the interface structures on the nucleation of lattice dislocations has been shown for grain boundaries in cubic [50–53] and hexagonal closed-packed [54–56] crystals, and in face centered cubic/body centered cubic (FCC/BCC) metallic nanolaminates [53–56]. For grain boundaries, lattice dislocations can form via dissociation of grain boundary dislocations that have a component of the Burgers vector pointing out of the interface plane [58–62]. On the other hand, in the atomic-flat FCC/BCC interfaces, cores of misfit dislocations that only have in-plane Burgers vectors, [16,63] extend in the interface, and consequently make dislocation nucleation difficult [8,16,64]. Zhang et al. [47,48] linked the dislocation nucleation mechanisms in Cu/Nb bi-layer system not only to the Schmid factor, but also to the structure of the intrinsic defects on the interface. They showed that the lattice dislocations favor nucleation from the interface dislocations that are parallel to the slip traces. Among multiple slip systems with highest Schmid factors, the one whose activation results in the formation of partial segment with the lowest self-energy is the most favored. In metal/ceramic multilayers, the nucleation initiates from the interface into the metallic layer that is more compliant than the ceramic layer[6,13]. Thus far, dislocation nucleation in multilayers has only been explored in the FCC layer of metallic FCC/BCC system where FCC crystal was the more compliant layer. Combination of metal and ceramic layers provides the opportunity to explore mechanisms of dislocation nucleation and propagation in a metal layer.

In this work, using molecular dynamics simulations, atomistically informed Frank-Bilby theory and disregistry analysis we first determined interface characters including the structures of

coherent interface regions and misfit dislocations in Nb/NbC multilayer as a representative metal/ceramic model. Then, we studied nucleation mechanisms of lattice dislocations from the Nb/NbC interface under two loading conditions: uniform compression and nanoindentation normal to the interface. We characterized nucleation mechanisms of lattice dislocations and analyzed the correlation of lattice dislocation nucleation with the interface structure. Finally we discussed how our characterization methods and results could be applied to other crystalline nano-laminated composites.

2. Atomistic Modeling

The Nb/NbC model adopts Baker-Nutting orientation relationship where $[100]_{\text{NbC}} \parallel [110]_{\text{Nb}}$ and $(001)_{\text{NbC}} \parallel (001)_{\text{Nb}}$ [37,65–69] (Fig. 1a). Using the second nearest neighbor modified embedded atom potential (2NN-MEAM) with the LAMMPS code [70], we explored the interface structure and the mechanisms of dislocation nucleation from the interface. MD simulations were carried out at 10 K. Simulations at low temperature assist understanding the deformation mechanisms due to less kinetic effects. The 2NN-MEAM potential is able to reproduce lattice parameters, enthalpy of formation, elastic properties, and surface energies of Nb and NbC [68]. This potential has been successfully applied to explore the plastic deformation and strain hardening in Nb/NbC multilayered composites [13]. Dahan and Dariel [71] explored the structural evolution of Nb/NbC multilayer coatings. They showed that annealing at temperatures higher than 600 °C would result in the formation of Nb₂C layer of 2-3 nm between the Nb and NbC layers. However, the presence of Nb₂C was not discernible at temperatures below 500 °C. Considering that Nb/NbC multilayers are fabricated by physical vapor deposition at 300~400 °C, a sharp interface will be obtained and thus the applied molecular dynamics model is valid.

To characterize the interface structure, a bi-layer model of NbC and Nb was assembled where the in-plane $\langle 100 \rangle_{\text{NbC}} \parallel \langle 110 \rangle_{\text{Nb}}$ directions are aligned to the x and z axes. Periodic boundary conditions were applied in all directions. Due to the lattice mismatch of 2.3% in both x and z directions, we chose the specific dimension of 20.0651 nm for both layers in x and z directions, corresponding to 44 units for NbC and 43 units for Nb. This results in the in-plane strains of 0.000052 for NbC and -0.000131 for Nb in both the x - and z -directions. Relaxed structure was obtained by energy minimization followed by quenching molecular dynamics at 10 K. Interface structure was studied using the disregistry analysis [14].

Two loading conditions including uniform compression and nanoindentation were considered in this work. Uniform compression helps us find the dominant dislocation nucleation mechanisms among all competing mechanisms related to the interface structure. Nanoindentation enables us to explore the mechanisms of dislocation nucleation from different regions of the interface due to the non-uniform stress field. Uniform compression loading was applied normal to the interface of the bi-layer model. The strain rate was $3 \times 10^{-8} \text{ s}^{-1}$.

Nanoindentation using a spherical tip was performed on a model that was periodic in the x and z directions and free in the y direction, that is normal to the interface (Fig. 1b). This model consisted of alternative 2 Nb layers and 2 NbC layers. The thickness of both Nb layers (in the bottom and at the middle of the model) was 6 nm, and both NbC layers were 2 nm thick. Various indenter sizes in the range of 40 nm-100 nm were considered to capture the main deformation mechanisms in relation to the indenter size. The indenter speed was 10 m/s. The deformation mechanisms and mechanical behavior of the model material were basically unchanged for lower indenter speeds [72,73].

3. Results and discussions

3.1. Interface structure

Arrays of misfit dislocations form in the interface as a result of the lattice mismatch between the adjacent layers to reduce the interfacial energy and consequently enhance the coherency [74]. More than one set of misfit dislocations exist and form the dislocation intersections that are also called nodes. It has been found that nodes affect the structure of misfit dislocations significantly [9,23]. Theoretical and numerical methods based on the linear elastic dislocation theory provide non-unique solutions for the characteristics of the misfit dislocation structure; therefore cannot fully capture the structure of the misfit dislocations. In addition, theoretical methods are not able to fully characterize the localized structures such as extended nodes on the interface [46,49,74–78]. To find the detailed structure of the interface, atomistic modeling using empirical interatomic potentials has been employed in this study.

According to the AIFB theory and disregistry analysis [14,76], the relaxed interface includes at least two orthogonal sets of edge dislocations [13,79], obvious coherent interface regions, and three complicated nodes (Fig. 2). The misfit dislocations in the interface are aligned to the plot of the disregistry vector in the interface, generated by comparing the relaxed structure to the unrelaxed structure. The solid dark-red and dark-blue lines in Fig. 2 represent the dislocation lines. The commensurate dichromatic pattern (CDP) lattice has the same crystallographic orientation as the Nb lattice [13]. The misfit dislocations are edge type with Burgers vectors $b_3 = \frac{\langle a \rangle}{2} [001]$ and $b_4 = \frac{\langle a \rangle}{2} [100]$ and the line senses along $[\bar{1}00]$ and $[001]$, respectively. One of the three nodes is condensed (marked in a star) and the other two nodes (marked with two different-sized squares) seem to form complex structures, which could be attributed to node reconstruction associated with misfit dislocations reactions[13,23,24]. In what follows, we report on a detailed

study of the interface structure including misfit dislocations, coherent interface regions, and nodes using disregistry analysis [14] and atomistic simulations.

Firstly, we studied possible coherent structures associated with atomic stacking sequences of the interface. The un-relaxed interface shows four types of stacks T1 to T4 (Fig. 3a,b). In T1 structure, Nb atoms in the Nb layer are located at the top of the Nb atoms in the NbC layer. In T3 structure, Nb atoms in the Nb layer are located at the top of C atoms in the NbC layer. If the Nb crystal in a T1 stacking region shifts along the vector $\mathbf{b}_1$ or $\mathbf{b}_2$ (defined in Fig. 3c), T2 structure forms where a Nb atom in the Nb crystal is located at the middle of the neighboring Nb and C atoms in the NbC layer. If the Nb crystal in a T1 stacking region shifts along the vector $\mathbf{b}_3$ or $\mathbf{b}_4$ (defined in Fig. 3c), T4 structure forms where a Nb atom in the Nb crystal is located at the center of a square outlined by two Nb and two C atoms in the NbC layer. During relaxation, the interface takes a low energy structure by balancing the energy of coherent interface regions, core energy of the misfit dislocations, and the node energy.

We thereafter calculated the interface energy of the four coherent Nb/NbC interfaces using molecular statics. Fig. 4 shows the interface energy surface. It is found that T1 structure has the highest interface energy (2.86 J/m^2) and is unstable. T3 structure has the lowest energy (1.88 J/m^2) and is the most stable. Experimental, first principles and MEAM calculations of the Fe/TiC (or TiN) interface also confirmed that regions with Fe atoms on the top of C (N) atoms are most energetically stable [69]. T4 structure is stable with the second lowest energy (1.99 J/m^2). T2 structure has the interface energy of 2.10 J/m^2 and interestingly exhibits a local energy minimum. Table 1 summarizes the structure and the energy of each coherent region in the interface. Fig. 4b shows the variation of interface energy with respect to the relative interface shift along $[110]$ ($\mathbf{p}_1$) and $[100]$ ($\mathbf{p}_2$) directions. The energy minima (marked by black arrows on the red curve) at T2

structure are evident. Thus it is expected that interface will form more T2 and T3 structures due to their low formation energy. This is consistent with our MD result (Fig. 5d).

Second, we explore the structure of misfit dislocations and dislocation nodes in the interface using the disregistry analysis [14,76]. The coherent interfaces with the aforementioned atomic stacks (T1, T3, and T4) have been chosen as the reference geometries to address the nodal/regional structures in detail. Starting from one of the T1, T3 or T4 structures, a relative shift of $\pm\mathbf{b}_1$ or $\pm\mathbf{b}_2$ yields the T2 structure. This relative shift can be represented by an interface dislocation loop with the Burgers vectors $\pm\mathbf{b}_1$ or $\pm\mathbf{b}_2$. Fig. 5a-c shows the disregistry analysis around different regions at the interface. The black lines denote interface dislocation loops enclosing the T2 regions. It is noted that there are four T2 regions surrounding each of the T1, T3 and T4 regions. Interface dislocation loops expand by reducing the chemical energy associated with the expansion of coherent interface structure and form the segmental misfit dislocations lines (dashed dark-red lines). The transition from the T1 or T3 structure to the T4 structure requires relative shifts along $\pm\mathbf{b}_3$ or $\pm\mathbf{b}_4$ vectors. Similarly such shifts are represented by the interface dislocation loops with Burgers vectors $\pm\mathbf{b}_3$ or $\pm\mathbf{b}_4$. Such loops are shown in the Fig. 5a-c using the solid brown lines. The disregistry plots (Fig. 5a-c) clearly reveal the structure of the nodes. Upon relaxation, the T1 structure was completely removed and a condensed node is formed (Fig. 5a). Both T3 and T4 regions remained intact and a set of segmental misfit dislocations (with burgers vectors $\pm\mathbf{b}_1$, $\pm\mathbf{b}_2$) surrounds each region (Fig. 5b, c). The relaxed interface contains large areas of T2 structure despite their shallow energy wells. Such observation might be attributed to the lower energy of the T2 structure compared to the core energy of equivalent dislocations if this region was removed. Having dislocation patterns around each coherent region, we then combine all the regions and find the misfit dislocations pattern on the interface (Fig. 5d). As shown in Fig. 5d, the interface structure includes the misfit dislocation

network (dashed dark-red lines), one condensed node, and three coherent interface structures (T2, T3, T4). Dislocation segments are edge type with Burgers vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ and $\mathbf{b}_4$. For the clarity of the display, we made the disregistry plots by comparing the relaxed interface with the un-relaxed interface.

3.2. Mechanisms of dislocation nucleation (and propagation)

Due to the formation of coherent interface structures and misfit dislocations, non-uniform strains develop in both crystals near the interface. The network of misfit dislocations on the Nb/NbC interface shows an array of strain concentrations that also serve as sources of lattice dislocation nucleation (Fig. 6). The strain analysis was performed for the first atomic layer of the Nb crystal adjacent to the interface, because the dislocation nucleation most likely commences in the Nb layer. Using the un-relaxed atomic structure as a reference configuration, the displacements of atoms in the first atomic layer of the Nb crystal during the relaxation process were first obtained. Then, treating each Nb atom as a node, the atomic displacement data were assigned to a triangular mesh with respect to the positions of the reference configuration. The strains for each element were calculated from the formulation for Constant Strain Triangle (CST) element in finite element analysis. The 2-D mean strain was therefore calculated as $\bar{\epsilon} = 0.5\epsilon_{ij}$, where $i = x, z$. To show smoother data, the 2-D mean strain was assigned to each node by averaging the values in the surrounding elements. The magnitude of the strain varies with the location on the interface, generally, high strain along misfit dislocation lines and/or at the condensed node. It is therefore expected that under deformation, these regions might be the preferred sites for the nucleation of lattice dislocations. In what follows, we studied the primary mechanisms for the nucleation of lattice dislocations from the Nb/NbC interface under a uniform

compressive loading, and also the secondary nucleation mechanisms using the highly non-uniform stress field generated by the nanoindentation.

(a) Uniform compression

Fig. 7 shows the atomic snapshots of successive nucleation and propagation of dislocation loops from the interface under uniform compression loading. Full dislocation loops nucleate from the condensed node. According to the mean strain analysis (Fig. 6), the condensed node region exhibits the highest strain concentration. Misfit dislocation lines across the condensed node are parallel to the traces of $\{110\}$ slip planes, and dislocations nucleate and propagate on these slip planes in the Nb layers (Fig. 7e). Nucleated dislocation resides on two different $\{110\}$ planes with the same Schmid factor, in the Nb layer. Two dislocations loops are annihilated at the intersection of the $\{110\}$ planes as they have the same Burgers vectors and the opposite line senses. Atomic snapshots shown in Fig. 7c and d indicate that these dislocations propagate and deposit in the interface, mainly in the T2 regions. It is also noted that the deposited dislocations do not necessarily follow the traces of misfit dislocations on the interface, indicating cross-slip has happened during the propagation.

(b) Nanoindentation

Simulations of uniform compression on the Nb/NbC sample showed that under constant stress field, dislocations preferentially nucleate from the misfit dislocations at the condensed nodes. To explore the mechanisms of dislocation nucleation from the defect structures at other regions in the interface, we performed nanoindentation on the Nb/NbC quad-layer sample (Fig. 1b).

Due to the non-uniform stress field under the spherical indenter, dislocation nucleation strongly depends on the location of the defect beneath the indenter. To study the effect of segmental misfit dislocations around the extended nodes on the dislocation nucleation, we positioned the indenter above the T3 region. For various indenter radii ranging from 40 to 100 nm, we observed the dislocation nucleation from the segmental partial dislocations surrounding the node at the region T3. Fig. 8 shows the mechanisms of dislocation nucleation from the interface into the Nb layer during nanoindentation with the tip radius of 50 nm. Since we are interested in early mechanisms of plastic deformation, the sample size is appropriate enough to assure that the boundary effects are minimum. The dislocation segments surrounding the T3 region are along the traces of $\{112\}$ slip planes in the Nb. Dislocations nucleate from one of the segments into a $\{112\}$ plane as shown in Fig. 8a. Then, dislocations cross slip on $\{110\}$ slip planes that intersect $\{112\}$ planes along $\langle 111 \rangle$ directions. Deposition of the dislocations along $\langle 100 \rangle$ direction (Fig. 8b, c) shows cross slip from $\{112\}$ planes to $\{110\}$ planes during deformation (Fig. 8a-c). These deformation mechanisms are schematically shown in Fig. 8d. If the indenter is sufficiently big, the stress field of the indenter can affect the dislocation segment connecting regions T3 and T4. The segment is along the trace of the $\{110\}$ plane. Therefore, lattice dislocations can nucleate from this interface dislocation segment. This dislocation is annotated as the secondary dislocation loop in Fig. 8c and it is also schematically shown in Fig. 8e.

Snapshots in Figs. 8b and 8c also show formation of vacancies during the deformation. These vacancies are the result of movement of sessile jogs. Fig. 9 shows the schematic of the vacancy formation. After the initial cross-slip of the dislocation loop on the $\{112\}$ plane (loops L1 or L2 in Fig. 9 a), subsequent cross-slips happen on other segments of the loop (loop L3, dashed line). The loops L3 and L2 reside on two parallel $\{110\}$ slip planes. The residual segment (colored in

cyan) left on $\{112\}$ slip plane is a jog that connects the two loops. The jog has the same Burgers vector ($b = \frac{a_{Nb}}{2}\langle 111 \rangle$) as the rest of the dislocation line (colored in blue), and is glissile within the $\{112\}$ slip plane. However, it is sessile in the $\{110\}$ slip planes. As shown in Fig. 9 b, under the resolved shear stress posed by the indenter, loops L2 and L3 bow out in $\langle 100 \rangle$ direction, marked by the red-yellow arrows. As a result, the jog is dragged in the $\{110\}$ plane by climb mechanism creating a series of vacancies. The jog also glides on the $\{112\}$ plane. Eventually the jog deposits into the top interface and loop L3 disappears. Hereafter, the motion of the loop L2 is pure glide and no more vacancies are created.

3.3 Discussions

Atomistic simulations and interface defect analyses have revealed that Nb/NbC interface adopts multiple stable coherent structures and holds a complicated interface misfit dislocation pattern. This is different from metal-metal interface where only one stable coherent interface exists and misfit dislocation pattern is relatively easy to be found [74]. In this work, we have proposed a method to identify the characteristics of the interface structure between a compound and a single element crystal. Step 1 is to identify possible coherent interface structures according to crystallographic analysis; Step 2 is to examine the stability of possible coherent structures; Step 3 is to characterize possible dislocation patterns with respect to a stable coherent structure; Step 4 is to compare these possible structures based on coherent interface energy and core energy of misfit dislocations. More importantly, the result implies a simplification of the above procedure. From the crystallographic analysis of the interface, a stable coherent interface structure that occupies the maximum area in the interface can be used as the primary reference structure for the analysis of the general interface dislocation pattern. As shown in Fig. 3a, energetically stable T2 coherent interface structure occupies half of the interface, and thus serves

as the primary reference structure. The other stable coherent interface structures can be used to reconstruct the structure of the nodal regions. This is evidenced by the experimental observation in MO/MgO laminates [65] where a square network of misfit dislocations with the periodicity of about 5.5 ± 0.5 nm was found. Mo/MgO interface adopts the same orientation relation as Nb/NbC interface and lattice mismatch between MgO and Mo (5.2 %) is close to that for Nb and NbC (2.3%). Due to the low resolution of the experimental technique, however, it is hard to identify whether misfit dislocation intersections are decomposed into a new coherent structure. In addition, atomistic simulations [23,24] and microscopic characterization [80] of semi-coherent fcc/fcc interfaces reported that misfit dislocation intersections could adopt different structures associated with the creation and reaction of interface dislocations, and such reconstruction of node structure is more obvious as the spacing between misfit dislocations or nodes is large [24]. Because of the small lattice mismatch (2.3%), the Nb/NbC interface has a large spacing of about 7 nm between the misfit dislocations, favoring node reconstruction.

For multilayers with the layer thickness in a few nanometers, plastic deformation is carried out by nucleation and emission of lattice dislocations from interfaces. Via molecular dynamics simulations, we have revealed a strong effect of interface structure on the position and type of lattice dislocations that nucleate from an interface into the adjoining crystal. Two activated slip systems $\{112\}\langle 111 \rangle$ and $\{110\}\langle 111 \rangle$ in Nb are observed in our atomistic simulations under two different loading conditions. The dislocation nucleation is preferred at the condensed node or along misfit dislocations that are parallel to the slip trace.

4. Conclusions

Molecular dynamics simulations using 2NN MEAM potential have been performed to explore the effect of interface structure on the inception of plastic deformation in Nb/NbC multilayer nanocomposites. Atomistic modeling examines interface-controlled nucleation behavior from atomically ordered bi-crystal interfaces, whose intrinsic defect structure can be described as a regular pattern of intersecting interface dislocations.

Using atomistically-informed Frank-Bilby (AIFB) method and the disregistry analysis, we characterized the structure of Nb/NbC interface, including misfit dislocations, dislocation nodes and three coherent interface structures. According to the crystallographic analysis on the interface, four possible coherent interface structures were identified, and three of them are energetically stable corresponding to the local energy minima. After relaxation of the interface, the unstable coherent interface region, which features Nb atoms in the Nb layer on the top of the Nb atoms in the NbC layer, evolves into a condensed interface dislocation node. The three stable coherent interface regions are associated with the formation, glide, and reaction of interface misfit dislocation loops. Disregistry analysis of the interface revealed that (a) all misfit dislocations are edge type and (b) misfit dislocations enclosing the coherent extended nodes have Burgers vectors along $\langle 110 \rangle_{\text{Nb}}$. We also proposed a crystallography-based method to identify the interface structure including the coherent regions and the misfit dislocations.

The role of the interface structure in plastic deformation of Nb/NbC nanolayered composites is studied under two loading conditions, i.e. uniform compression and nanoindentation. Under uniform compression, dislocations primarily nucleate from the condensed nodal regions where the local strains are the highest. These dislocations propagate in two $\{110\}$ slip planes in the Nb layers with the same Schmid factors. Under nanoindentation, by proper positioning of the indenter, dislocations nucleate from the segments of the misfit dislocations and propagate in

{112} slip planes in the Nb layers. Simulations also show the cross slip from {112} planes into {110} planes and the formation of vacancies as a result of climb of dislocation jogs. This work examines interface-controlled nucleation behavior from atomically ordered metal/ceramic interface, whose intrinsic defect structure can be described as a regular pattern of intersecting interface dislocations. It is observed that dislocations nucleate on the nodes and misfit dislocations.

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Figure Captions

Figure 1- (a) Baker-Nutting orientation relationship ($[100]_{\text{NbC}} \parallel [110]_{\text{Nb}}$ and $(001)_{\text{NbC}} \parallel (001)_{\text{Nb}}$) in Nb/NbC interface. Nb Atoms in the Nb layer are colored yellow, Nb atoms in the NbC layer are colored red and C atoms in the NbC layer are colored blue. (b) The simulation cell used in the nanoindentation loading.

Figure 2- Disregistry plot of the relaxed NbC/Nb interface. Dislocation structure of the Nb/NbC interface is shown in solid dark-red and dark-blue lines. A star and two squares enclose three types of nodes. The disregistry vectors are shown with the magnification factor of 18. The average dislocation spacing is 7 nm.

Figure 3- (a) The un-relaxed Nb/NbC interface. The dashed square shows the super-unit cell of the interface. Locations of coherent interface structures type 1(T1)-type 4(T4) are indicated. (b) Four coherent interface structures T1-T4. (c) Four possible Burgers vectors that are defined in the reference lattice. Nb (red dots) and C (blue dots) are added for further clarification.

Figure 4. (a) The interface excess energy surface of the coherent Nb/NbC interface. (b) Profile of the interface excess energy along the vectors p_1 (the $[110]$ direction) and p_2 (the $[100]$ direction). Both horizontal axes are normalized by the b_1 and b_4 vectors respectively, which align with the vectors p_1 and p_2 . Arrows show the local minima corresponding to the T2 structure.

Figure 5- Disregistry plots of Nb/NbC interface showing dislocation structures around (a) T1 region, (b) T3 region, (c) T4 region. The reference configuration was chosen as the coherent stacking for each region. (d) Disregistry plot on the entire interface with T1 stacking as the reference. The plots are colored according to the magnitude of the disregistry.

Figure 6- Contour plot of the mean strain in the first atomic layer of the Nb crystal adjacent to the Nb/NbC interface, showing the highest strain at the condensed node (the un-relaxed T1 region).

Figure 7- Mechanisms of dislocation nucleation from the Nb/NbC interface and dislocation propagation into the Nb layer under uniform compression loading. (a) Dislocations nucleate at the condensed node in two $\{110\}$ slip planes. (b-d) Dislocations propagate and deposit on the T2 region in the interface. Atoms are colored according to the y coordinate. (e) Schematic of dislocation nucleation from the misfit dislocations at T1 region in two $\{110\}$ slip planes and dislocations propagation in the two $\{110\}$ slip planes. Dislocation loops are being annihilated at the intersection of the two slip planes. OVITO was used to visualize the atomic snapshots in this work [81].

Figure 8- (a-c) atomic snapshots showing mechanisms of dislocation nucleation and propagation in Nb/NbC sample under nanoindentation with the tip radius of 50 nm. (a) Primary dislocation loop nucleates from a misfit dislocation segment around T3 region and glide in $\{112\}$ plane. (b-c) cross slip of the dislocation loop into $\{110\}$ planes. The trace of the deposited dislocation is parallel to $\langle 100 \rangle$ direction on the interface, indicating the cross slip of the dislocation. Atoms are colored according to the y coordinate. (d) Schematic of the primary deformation mechanisms in the Nb/NbC sample under nanoindentation. (e) Schematic of the nucleation of the secondary dislocation loop that forms on $\langle 100 \rangle$ dislocation line and glides on $\{110\}$ slip plane in the Nb layer.

Figure 9- The schematic illustrating the process of the vacancy formation. (a) The nucleated dislocation loop cross-slips into two parallel slip planes, loop L2 on $\{110\}$ -1 and loop L3 on

$\{110\}$ -2, forming the jog (colored cyan). (b) A series of vacancies are left behind the moving jog. The jog eventually glides on $\{112\}$ plane and deposits on the top interface.

Table 1- Structure and energy of coherent regions in Nb/NbC interface

Atomic stacking	Relative positions of atoms on the interface	Interface energy (J/m ²)
T1	Nb atom in Nb on the top of Nb atom in NbC	2.86
T2	Nb atom in Nb on-between the neighboring Nb and C atoms in NbC	2.1
T3	Nb atom in Nb on the top of C atom in NbC	1.88
T4	Nb atom in Nb on the center of a square outlined by two Nb atoms and two C atoms in NbC	1.99