University of Nevada, Reno

Understanding the Atomistic Deformation Mechanisms of Cu-Nb Multilayered Nanocomposites using Molecular Dynamics

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Abstract

Metal-metal multilayered nanocomposites exhibit a remarkable improvement in strength, thermal stability, and irradiation resistance. This superior response of multilayered nanocomposites is attributed to various factors, such as the high density of interfaces, layer thickness, and nature of interfaces. In the current work, molecular dynamic simulations will be utilized to study the uniaxial (tension and compression) mechanical response of Cu-Nb multilayered nanocomposites (MNCs). In specific, the aim is to understand the deformation mechanisms of accumulative roll bonded vs. physical vapor deposited interfaces with nanolayered Cu and Nb. In addition, the effect of loading mode (tension vs. compression) and crystallography on the deformation of MNCs is discussed in detail with emphasis on atomic-scale interactions between dislocations, dislocation-interfaces, and dislocations-twins. The outcome of this work would serve as a supplement to plasticity literature which provides deep insights into interfacial deformation mechanisms and defect formation in metal-metal multilayered nancomposite under various loading scenarios.
Dedication

This work is dedicated to the countless efforts of all the warriors during this COVID pandemic in the service of humanity.
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Nomenclature

\( \sigma_{ys} \)  Yield strength
\( h \)  Layer thickness
\( \tau_{CLS} \)  Confined layer strength
\( \varphi \)  Chemical Potential

\( \langle A \rangle_{ensemble} \)  Statistical average

\( P(v_{ix}) \)  Potential energy as a function of velocity

\( F_{\varphi_i} \)  Embedding energy of atom type \( \varphi \) with an index \( i \)

\( E_{iso-stress} \)  Elastic modulus under iso-stress loading

\( E_{Cu} \)  Elastic modulus of copper

\( E_{Nb} \)  Elastic Modulus of Niobium

\( T \)  Temperature

\( \rho \)  Probability density of the ensemble

\( Q \)  Partition function

\( \overrightarrow{R_i} \)  A vector from atom I to its neighbors

\( b \)  Burgers vector

\( K_B \)  Boltzmann constant

\( V_{\varphi_i\varphi_j} \)  Pairwise interaction energy

\( k \)  Hall-Petch slope

\( H \)  Hamiltonian

\( N \)  Number of particles
Chapter 1: Introduction

1.1 Motivation and Overview

Two-phase nanolayered composites with individual layer thicknesses varying from 200-300 nm down to 1-2 nm have been the subject of vigorous study because of their unusual physical, chemical, and mechanical properties [1-12]. Multilayered nanocomposites have been extensively studied for a wide range of mechanical, thermal, and nuclear applications due to their very high strength, considerable ductility, thermal stability, and radiation resistance [13-15]. Moreover, if the constituent phases present significant differences in the strength, elastic modulus, and ductility, these multilayers give rise to new possibilities for the deformation mechanisms and properties of the composite as a whole.

1.1.1 Interfaces present in MNCs

MNCs have a high density of interfaces; for example, nanocomposites with individual layers of 5 nm will have 1000 interfaces in a 5 μm sample. These interfaces have been shown to play a significant role during the deformation of MNCs with different length scales of interface spacings. Dislocation activities involving pile-up at the interface leading to Hall-Petch type of strengthening, confined layer slip strengthening, and single transmission of dislocation across the interfaces (softening stage) (see Fig 1.1) [24-30]. The atomic structure of interfaces in MNCs depends on the processing route. For example, Cu-Nb MNCs manufactured via PVD have atomically sharp interfaces with Kurdjumov–Sachs (K-S) Cu {111}‖Nb {110} orientation relationship [16]. The Cu-Nb interfaces as fabricated by ARB have faceted K-S interfaces with Cu {112}‖ Nb {112}
orientation relationship [17]. Changes in the interface structure and/or layer thickness could indicate a transition in the strengthening mechanisms from conventional polycrystal plasticity to a confined layer slip to dislocation transmission across the interface [18,19]. In general, the ARB processed Cu-Nb sample has K-S Cu $\{112\}$\$\{112\}$ with Cu $\{111\}$\$\{110\}$ orientation relationship along the lateral direction. This crystallographic orientation gives rise to the anisotropic mechanical properties of the MNCs. In general, MNCs are synthesized using atom-by-atom deposition methods such as physical vapor deposition (PVD) [16-20] and bulk manufacturing techniques such as accumulative roll bonding (ARB) [21-23]. A myriad number of works over the past years involving atomic-scale investigations and dislocation theory have been dedicated to studying the role of interfaces in controlling the dislocation motion in MNCs under deformation [11, 21], [24–30]. In addition, interfaces have been shown to act as

**Figure 1.1** Nucleation of a single Shockley partial dislocation under in-plane shear.

This loop was induced by stress concentrations in the interface generated around a misfit under the applied strain state [36].
dislocation nucleation sources, sink for incoming radiation, dislocation barrier, and dislocation or twin repository [11, 21, 31, 32]. The atomic structure of interfaces in MNCs depends on the processing route. For example, Cu-Nb MNCs manufactured via PVD have atomically sharp interfaces with Kurdjumov–Sachs (K-S) Cu \{111\}‖ Nb \{110\} orientation relationship [33]. The Cu-Nb interfaces as fabricated by ARB have faceted K-S interfaces with Cu \{112\}‖ Nb \{112\} orientation relationship [34]. Changes in the interface structure and/or layer thickness could indicate a transition in the strengthening mechanisms from conventional polycrystal plasticity to a confined layer slip to dislocation transmission across the interface [4-6], [35-36]. The process of dislocation nucleation and its relation to interface pattern has been explored by atomistic simulations, as shown in Fig 1.2 [23, 27].

1.1.2 Mechanical properties of MNCs

The dislocation nucleates at the interface into a layer of the nanocomposite which has a slip system with the highest resolved shear stress [37–39]. The nucleated dislocation either glides across the layer and deposits at the adjacent interface or transmits across the interface into another layer. However, the latter requires higher energy [40].

The strength of MNCs majorly depends on the layer thickness. The size effect on strength due to layer thickness has been observed in experimental and computational means [5,6]. The schematic in Fig. 1.2 illustrates this effect, when the layer thickness is in the range of micrometers to hundreds of nanometers, the strengthening of MNCs is governed by the
traditional Hall-Petch relationship [5], where dislocations pile up at the interfaces and strengthening is guided by Eq. (1.1).

\[ \sigma_{ys} = \sigma_0 + kh^{-0.5} \]  

(1.1)

where \( k \) is the Hall-Petch slope and \( \sigma_0 \) is the lattice fraction stress to slip.

When the layer thickness of MNCs is reduced to a few nanometers to tens of nanometers, the strengthening occurs by a mechanism called confined layer slip, where dislocations bow within the individual layer (see Fig. 1.2.). Dislocation bowing via confined layer slip model can be predicted by Eq. (1.2).

\[ \tau_{CLS} = \frac{\mu b \sin \Theta}{8 \pi h} (4 - \nu) (1 - \nu) \ln \left( \frac{ah}{b \sin \Theta} \right) \]  

(1.1)

where \( h \) is the film thickness, \( \mu \) is the shear modulus, \( \nu \) is the Poisson's ratio, \( \Theta \) is the angle between a slip plane and an interface plane, \( b \) is the Burgers vector, and \( \alpha \) represent the dislocation core cutoff parameter (Low values of \( \alpha \) imply a wide dislocation core).

From Eq. (1.2), the critical stress dependence on layer thickness is proportional to \( \ln(h)/h \).

When the layer thickness is reduced to 1-2 nm, the deformation occurs via single transmission of dislocation across the interface.

Another important property of MNCs is the toughness dictated by strength and ductility. The interfaces in MNCs greatly influence both the strength and ductility and also control the fracture mechanisms. Fracture mechanisms in MNCs made of Cu-Ta were investigated by Zhu et al. [41]. Their study showed that below a critical layer thickness, the fracture mode of the MNCs is governed by the shearing failure. The fracture behavior of MNCs made of Cu-Nb and Cu-Zr was studied by Zheng et al. [42]. Their experimental
mechanical testing results showed that when the layer thickness of the Cu layer was reduced below 60nm, the failure mechanism transitioned from brittle fracture to shear fracture, as illustrated in Fig. 1.3. This transitioning of fracture modes is dominated by the deformation of the soft Cu layer. The in-situ TEM fracture mechanics study by Hattar [43] et al. indicated four fracture steps during the crack propagation stage in Cu-Nb, as shown in Fig. 1.4. A study by Liang et al. [44] also indicated the transitioning of fracture mechanisms from brittle mode to necking delayed ductile mode in Cu-Ni MNCs when the layer thickness of Ni was reduced from 90nm to 40nm.

Another important factor that governs the deformation mechanisms is the 3-dimensional crystallographic orientation of the MNCs and the mode of loading (tensile vs. compression). The crystallographic orientation gives rise to the anisotropic mechanical properties of the MNCs. Furthermore, nanocrystalline Cu exhibits asymmetry in tension and compression plastic deformation [45-46]. Molecular dynamics study of Cu nanowires showed that deformation mechanisms in Cu were highly influenced by the crystallographic orientation and mode of loading [47]. In particular, it was shown that the orientations close to the <100> corner of the stereographic triangle were deformed by twinning, and those that are away from <100> deformed via full dislocation slip under compressive loading. On the contrary, orientations close to <111> position of stereographic projection were deformed via twinning under tension and dislocation slip under compression. This asymmetric behavior was attributed to different Schmid factor values for leading partial dislocations under tension and compression loading. Despite the
vast body of work on MNCs, the detailed investigation on the effect of crystallography and the loading direction on the deformation mechanisms still need to be elucidated.

\[ \sigma \neq f(h) \]

\[ \sigma \propto -\frac{\ln(h/b)}{h} \]

\[ \sigma \propto h^{-1/2} \]

**Figure 1.2** Schematic showing dependence of yield strength and deformation mechanisms as a function of layer thickness [6].
Figure 1.3 Fracture models observed and developed by Zhang et al. [42] (a) Opening fracture model with larger layer thickness (b) Ductile type shear fracture with small layer thickness.

Figure 1.4 Four crack hindrance processes during crack propagation found by Hattar et al. [43] (a) micro-void; (b) crack deviation; (c) layer necking; (d) crack blunting
1.2 Research focus

The focus of this work is to explore the role of interfaces, crystallography, and mode of loading on the atomic scale deformation mechanisms of PVD and ARB processed Cu-Nb MNCs. Emphasis is put on understanding the interaction between dislocations, interfaces, and twins in the MNCs.

The versatile Molecular Dynamics modeling approach has been applied in this study to elucidate the effect of interface orientation, loading mode, and crystallography on the deformation mechanisms of Cu-Nb multilayered nanocomposites. Molecular dynamics simulations of deformation behavior of accumulative roll bonding and physical vapor deposited Cu-Nb multilayered nanocomposites (MNCs) were performed at room temperature conditions and a constant strain rate under iso-stress and iso-strain conditions. The simulations were explored to understand the elastic, yield, and post-yielding behavior of Cu-Nb MNCs. Interface deformation mechanisms involving nucleation of partial dislocation at the interface and gliding in the Cu layer were observed under both iso-stress and iso-strain conditions.

1.3 Thesis layout

The analytical concept of the molecular dynamics simulations for investigating deformation mechanisms of MNCs is summarized in Chapter 2. In the second part of this section, descriptions of the necessary model equations and their associate numerical implementations are presented. The details of the simulation geometry and setup are also described in Chapter 2, followed by the definition and selection of the critical parameters for the modeling approach that has been presented in the previous chapter.
Chapter 3 focuses on understanding the structure and properties of accumulative roll bonding (ARB) interfaces using molecular dynamics. An atomic-scale phenomenon related to deformation mechanisms is investigated using molecular dynamics under tension and compression. The effect of loading normal to the interfaces (iso-stress) and parallel to the interfaces were discussed. The effect of crystallography on the mechanical response of multilayered nanocomposites has been the focus of Chapter 3.

Chapter 4 deals with the mechanical deformation studies of Physical Vapor Deposited Cu-Nb interfaces. The process of physical vapor deposition and the type of interfaces formed during this processing technique is described in this chapter. Loading scenarios similar to chapter 3 has been explored to understand and contrast the Effect of PVD and ARB interfaces on the mechanical response of Cu-Nb multilayered nanocomposites.

Chapter 5 discusses the conclusions drawn from the deformation study conducted on multilayered nanocomposites using atomistic modeling.
Chapter 2: Simulation Method: Molecular Dynamics

2.1 Introduction

Molecular dynamics (MD) and Density Functional Theory (DFT) are widely established methods used to study atomic-scale mechanisms. DFT [48] modeling is used when the length scales are in the range of angstrom to a few tens of nanometer, whereas MD [49] is used to predict material properties on the length scale of a few angstroms up to 100nm. MD simulations represent a technique that produces solutions of many-body interaction at an atomic scale [50–54].

MD has proven to be a promising tool to study the deformation behavior of crystalline materials [55,56]. It can predict atomic-scale phenomenon such as dislocation nucleation [57], multiplication [58] and dislocation-dislocation [59], and dislocation-twin interactions [59] during the deformation. In an MD model, a three-dimensional coordinate space is occupied by atoms which are specified by local symmetry representing a particular crystal structure such as face-centered cubic (FCC), body-centered cubic (BCC). The core of the MD simulation depends on the interatomic potentials function assigned to each atom [60]. Interatomic potentials predict the potential energy of a system of atoms with given positions in space [61]. The predicted potential energy can then be used to calculate properties such as the force on an atom, stress, pressure, and temperature, etc. Another important aspect in running an MD simulation lies with the boundary conditions applied to the system. Boundary conditions include surface boundaries, grain boundaries, interphase boundaries, and periodic boundaries to ensure crystalline continuity. Thermostats based on Nose- Hoover [62] are used to
control the temperature, and appropriate pressure is selected to calculate the new position of each atom prior to the start of the simulation run.

Deformation studies using MD simulations are performed by displacement of a plane of boundary atoms by the application of the required strain rate. The strain rate induces displacement and re-evaluation of the position of each atom in every time step, which is in the range of Femto seconds $10^{-15}$ S. For example, to achieve 2% elongation at a strain rate of $10^8$ S$^{-1}$, the total number of calculation steps required is 200,000. At each time step, the forces on each atom including the internal forces generated by surrounding atoms within a 5 nm distance. The outcome of these forces is a velocity vector that can be used to calculate the new position of each atom, including other parameters such as stress state, energy, and temperature of the system at each time step.

Post-processing after the simulation run generates the coordination of atoms and their neighboring atoms to identify the local crystal type and show both planar (Stacking Faults) and linear defects (dislocations) [63]. The microstructural evolution during the deformation can be visualized using software such as Ovito [64]. Despite being a versatile technique to predict material behavior, MD simulations offer key challenges with respect to computational time. In addition, the simulation box is currently limited to 100 nm length scales which uses 128 CPUs (Central Processing Units) and requires a week's time for completion of the run. Another limitation of MD simulation lies with the time step, which should be in the range of femto seconds to satisfy the range of atomic frequency in the system. This inherent time step limitation makes MD simulations run at
thousands of times the quasistatic strain rates, presenting a significant hurdle for direct comparison between the MD and the experimental results.

Many codes and algorithms have been developed to implement the MD simulations [45]. In this work, the LAMMPS (Large-scale-Atomic/Molecular Massively Parallel Simulator) code is used [45]. LAMMPS is a versatile tool that can be used to run either a single processor or in parallel multiple CPU clusters.

2.2 Ensemble, Boundary Conditions, and Loading Method

The microscopic of the system containing 'N' particles is defined by the atomic positions' q's and their momenta' p.' These positions and momenta of particles are represented as coordinates in a multidimensional space called phase space. An ensemble of a system is a collection of points in phase space satisfying a particular thermodynamic or macroscopic state and may have different microstates [65]. Three main ensembles exist having different characteristics, namely,

1. Microcanonical ensemble (NVE) – Thermodynamic state defined by a fixed number of atoms, 'N,' a fixed volume, 'V,' and fixed energy, 'E' making it an isolated system where the energy of the system cannot be changed with respect to its surroundings.

2. Canonical Ensemble (NVT) – In this ensemble, the thermodynamic state of the system is described by a constant number of particles, 'N,' constant volume, 'V,' and fixed temperature, 'T.'
3. Isobaric-Isothermal ensemble (NPT) – This thermodynamic state of this ensemble is represented by a fixed number of atoms' N', fixed temperature 'T,' and fixed pressure 'P'.

4. Grand Canonical Ensemble (ϕVT) – This ensemble contains a fixed chemical potential, 'ϕ,' fixed volume, 'V' and fixed temperature, 'T.'

Calculating Averages from Molecular Dynamic simulations: In statistical mechanics, averages corresponding to ensemble averages taken over a large number of replicas of the system are considered simultaneously [65] is given by Eq. (2.1).

\[
<A>_{ensemble} = \int \int dp^N dr^N A(p^N, r^N) \rho(p^N, r^N)
\]

(2.1)

Where, \( A(p^N, r^N) \) is the property of interest as a function of momenta, 'p,' and the positions, 'r' of the system.

The probability density of the ensemble is given by Eq. (2.2),

\[
\rho(p^N, r^N) = \frac{1}{Q} exp[-H(p^N, r^N)/K_B T]
\]

(2.2)

Where \( H \) is the Hamiltonian, \( T \) is the temperature, \( K_B \) is Boltzmann's constant, and \( Q \) is the partition function given by Eq. (2.3),

\[
Q = \int \int dp^N dr^N exp[-H(p^N, r^N)/K_B T]
\]

(2.3)
In MD, these statistical averages are calculated as a function of time sequentially corresponding to the particular thermodynamic condition given by Eq. (2.4).

\[
< A >_{time} = \lim_{\tau \to \infty} \left( \frac{1}{\tau} \right) \int_{t=0}^{\tau} A (p^N(t), r^N(t)) \, dt \approx \frac{1}{M} \sum_{t=1}^{M} A (p^N, r^N) \tag{2.4}
\]

Where \( \tau \) is the simulation time, and \( M \) is the number of time steps in the simulation and \( A(p^N, r^N) \) is the instantaneous value of measurable quantity 'A.'

Under the assumption of the Ergodic hypothesis, which implies that when the system is allowed to evolve over indefinite time, the system will eventually pass through all possible states making times averages equal to the ensemble averages. For example, considering the above assumption, the average potential energy of the system can be by Eq. (2.5).

\[
P = < P > = \frac{1}{M} \sum_{i=1}^{M} P_i \tag{2.5}
\]

Where \( M \) is the number of trajectories in the MD run, \( P_i \) is the potential energy of each configuration.

**Boundary Conditions (BC):** Boundary conditions are an important part of MD simulations. In general, there are three different types of BC used.

1. **Free Surface BC:** Under the Free Surface BC, the space outside the surface layer of atoms is treated as a vacuum. Frees surface boundary conditions are especially
useful in calculating the surface mechanisms such as free energy of the surface (E.g., Stacking Fault Energy), the interaction between salts and interfaces. Fig. 2.1 shows the free surface boundary condition applied along the Y direction.

2. Fixed Boundary Condition: Fixed boundary condition ensures the rigidity of the surface layer of atoms which makes them immobile, as shown in Fig. 2.1 along the X-direction.

3. Periodic Boundary Condition (PBC) – Periodic boundary condition connects the atoms from one side to the other side, ensuring the periodicity across two surfaces. In Fig. 2.1, the central portion of the simulation box is under PBC. It is one of the common BCs used in MD simulations as it reduces the number of

**Figure 2.1 Schematic of free surface BC along the Y direction, rigid BC along the X-direction and PBC in X direction.**
atoms in the system and thus reducing the computational time.

**Loading Method:** MD simulations have been used to explore the atomic scale deformation mechanisms [66]. The deformation of the system can be explored by applying a strain to the sample. The strain can be applied either uniaxially or biaxially on the simulation box incrementally at each time step. The new coordinates of atoms are then recalculated inside the simulation box.

### 2.2.1 The Interactive Potential

In MD simulations, the interaction between the atoms is calculated by the interactive potentials. The interatomic potential has both attractive and repulsive components depending on the binding nature of atoms. The accurate interatomic potential requires high computational power, e.g., thousands of CPUs and thousands of hours. The efficiency of the simulation can be improved by using the approximate empirical interaction potentials, e.g., Leonard-Jones potentials, Tersoff potentials, Embedded-Atom Method (EAM) potentials [67]. Simple pair-potentials like that of Leonard-Jones potentials are not as good as the many-body embedding functional potentials like EAM potentials. Furthermore, EAM potentials have proven sufficiently accurate for studying FCC and, to a lesser degree, BCC metals [68-70]. The total energy of the system described by an EAM potential contains: the embedding energy $F_{\kappa_i}$ and a pairwise interaction energy $V_{\kappa_i \kappa_j}$ given by Eq. (2.6),
\[ E_{\text{total}} = \sum_i \left[ F_{\alpha_i} \left( \sum_{j \neq i} \rho_{\alpha_j}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} V_{\alpha_i\alpha_j}(r_{ij}) \right] \]  \hspace{1cm} (2.6)

Where subscript \( \alpha_i \) represents the type of atom with index \( i \), \( \rho_{\alpha_j} \) is the electron density function for atom type \( \alpha_j \) and \( r_{ij} \) is the distance between atoms \( i \) and \( j \).

The Cu-Nb interatomic potentials used in this study are adapted from the work of Zhang et al. [104], which are of EAM type and predicted the phase diagram of the Cu-Nb system, which is closely matched with experiments.

### 2.2.2 Numerical implementation

The equations of the MD simulations are solved using Newton's second law of motion, which states that the force '\( F \)' exerted on a particle is directly proportional to its mass '\( m \)' and acceleration ‘\( a \)’ given by \( F = m \cdot a \). Integration of the equations of motion yields a velocity and a position vector which vary with time. From this trajectory, required properties of interest can then be calculated as averages as approximated by the Ergodic hypothesis [68].

Numerical implementation of MD simulations based on Newtonian mechanics is explained as follows [66]: The force equation from Newton’s second law of motion is given by Eq. (2.7),

\[ F = m \cdot a = m \frac{dv}{dt} = m \frac{d^2x}{dt^2} \]  \hspace{1cm} (2.7)
Considering the simple case where the acceleration is constant, as given by Eq. (2.8),

\[ a = \frac{dv}{dt} \quad (2.8) \]

Integrating the acceleration of Eq. (2.8), velocity can be obtained by Eq. (2.9),

\[ v = a \cdot t + v_o \quad (2.9) \]

The position of a particle as a function of acceleration, initial velocity \( v_0 \), initial position \( x_0 \), and time \( t \) is given by Eq. (2.10),

\[ x = 0.5 \cdot a \cdot t^2 + v_0 \cdot t + x_0 \quad (2.10) \]

The acceleration can be calculated as a gradient of energy of particle with respect to its position, given by Eq. (2.11),

\[ a = -\frac{1}{m} \frac{dE}{dr} \quad (2.11) \]

Thus, the trajectory of atoms in the system can be calculated by knowing the initial velocities, initial positions. The initial velocities can be obtained from Maxwell-Boltzmann or Gaussian distribution at a given temperature, which gives the probability of velocity of an atom \( i \) along the X direction at temperature \( T \) considering that there is no overall momentum for a system of \( N \) number of atoms given by Eq. (2.12) and Eq. (2.13).

\[ P = \sum_{i}^{N} m_i v_i \quad (2.12) \]
\[ P(v_{lx}) = \left( \frac{m_i}{2\pi k_B T} \right)^{0.5} \exp \left[ -0.5 \frac{m_i v_{lx}^2}{k_B T} \right] \] (2.13)

The temperature can be calculated from the velocities as below Eq. (2.14)

\[ T = \frac{1}{(3N)} \sum_{i=1}^{N} \frac{p_i}{2m_i} \] (2.14)

**Integration Algorithms:** The integration algorithms used the Taylor series approximation as follows given by Eq. (2.15), (2.16), and (2.16).

\[ r(t + \delta t) = r(t) + v(t) \delta t + \frac{1}{2} a(t) \delta t^2 + \ldots. \] (2.15)

\[ v(t + \delta t) = v(t) + a(t) \delta t + \frac{1}{2} b(t) \delta t^2 + \ldots. \] (2.16)

\[ a(t + \delta t) = a(t) + b(t) \delta t + \ldots. \] (2.17)

Where \( r \) is the position, \( v \) is the velocity, and \( a \) is the acceleration.

Verlet algorithm can be derived as follows:

\[ r(t + \delta t) = r(t) + v(t) \delta t + \frac{1}{2} a(t) \delta t^2 \] (2.18)

\[ v(t + \delta t) = v(t) + a(t) \delta t + \frac{1}{2} b(t) \delta t^2 + \ldots. \] (2.19)

Adding equations 2.14 and 2.15

\[ v(t + \delta r(t + \delta t)) = 2r(t) - r(t - \delta t) + a(t) \delta t^2 \] (2.20)

The above algorithm uses positions \( r(t) \) at time \( t \) and \( r(t-\delta t) \) from time \( t-\delta t \) to calculate new position \( r(t+\delta t) \) at time \( t+\delta t \).
2.3 Model construction of accumulative roll bonded Cu-Nb nanocomposites

2.3.1 Analysis of atomic interface structure

The molecular dynamics (MD) simulations of Cu-Nb multilayered composites (MC) were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) under embedded atom method potential [45]. The Ovito software [64] was utilized to visualize MD trajectory data after deformation under uniaxial tension and compression of strain rate (3×10^8 s^{-1}). The temperature of the system was controlled using a Nose-Hover thermostat [62].

The Cu-Nb interfaces under investigation were constructed in a bilayer fashion [10]. The bilayer consisted of {112} face-centered cubic (FCC) Cu connected to free surface of a {112} body-centered cubic (BCC) Nb. A total of 54-unit cells of Cu were stacked over a 76-unit cell of Nb to obtain a Cu-Nb bilayer of 8nm/8nm layer thickness. The Cu-Nb bilayer cross-section parallel to the interface is a rectangle with dimensions 4 nm by 7 nm. To ensure periodicity in the interface plane, the plain strain was applied to one of the adjoining layers. The shape and dimensions of the Cu-Nb layers were chosen such that this strain is minimized. Due to crystal structure mismatch between Cu and Nb, misfit dislocations were observed extending into the Cu layer as indicated by the white circles and ellipses. Similar observations were also recorded in the molecular dynamics study by Kang et al. [69].
2.3.2 PVD model of Cu-Nb nanocomposites

Multilayered nanocomposites (MNCs) with nanolayers are fabricated via physical vapor deposition (PVD). Previous atomistic simulations and electron microscopy experiments on PVD deposited Cu-Nb MNCs have shown to have FCC Cu \{111\} \parallel BCC Nb \{110\} interface orientation. The Cu-Nb MNCs in this study were fabricated in a bilayer fashion by joining FCC Cu \{111\} to BCC Nb \{110\}. The volume fractions of Cu and Nb are equal with an individual layer thickness of 5nm. Periodic boundary conditions were applied to all three dimensions to ensure the connectivity between the layers forming a multilayered structure and to reduce the number of atoms in the system. The above structure was produced using Atomsk software [70].

MD simulations were performed using a Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) under embedded atom method potential. The Ovito software was utilized to visualize MD trajectory data after deformation under uniaxial tension and compression of strain rate \(3\times10^8\ \text{s}^{-1}\). The temperature of the system was controlled using Nose- Hoover thermostat. The system was equilibrated first by applying energy minimization at 0K until the maximum force on any atom was smaller than \(1\times10^{-10}\ \text{N}\).

2.4 Post-Processing: Visualization of MD Trajectory

The microstructural evolution during the deformation of Cu-Nb nanocomposites can be better understood when the visualization technique is used to view the trajectory of the system. Post-processing tools can also provide independent parameters such as Centro-
Symmetric Parameter (CSP) [71] and a Common Neighbor Analysis (CNA) [72] parameter. Furthermore, microstructural defects that emerge during uniaxial compression and tension, such as dislocations, twin boundary, interface dynamics, and stacking faults, can be easily observed, and identified. The CSP parameters are commonly used parameters in the post-processing of the MD simulation for visualizing planar faults in FCC and BCC crystals [73]. The CSP is computed by:

$$P = \sum_{i=1}^{N/2} |\vec{R}_i + \vec{R}_{i+N/2}|$$  \hspace{1cm} (2.21)

Where, $\vec{R}_i$ is a vector from atom I to its neighbors, and N is the number of neighbors. For an FCC crystal, N=12, and for the BCC structure, N=8.

Atomic-scale plastic deformation mechanisms can be identified using post-processing tools. Different plastic activities including dislocation slip, dislocation nucleation, the interaction between dislocations-twin boundary, and interaction between dislocation and interface. Comparing the relative motion between nearest neighbors of each atom before

![Figure 2.2 Schematic of slip of atom A with respect to atom B.](image)
and after the deformation yields defect structure generated as shown in Fig. 2.2.

The relative distance between atom A and atom B can be obtained using Eq. 2.21.

\[ \overrightarrow{d_{int}} = (X_A^0 - X_B^0, Y_A^0 - Y_B^0, Z_A^0 - Z_B^0), \]

where \( \overrightarrow{d_{int}} \) is the displacement vector before deformation, \( X_A^0 \) is the initial X-coordinate of atom A and \( X_B^0 \) is the X-coordinate of atom B. \( Y_A^0, Y_B^0 \) and \( Z_A^0 \) and \( Z_B^0 \) are the Y and Z coordinates of atoms A and B, respectively.

\[ \overrightarrow{d_{def}} = (X_A' - X_B', Y_A' - Y_B', Z_A' - Z_B'), \]

where \( \overrightarrow{d_{def}} \) is the displacement vector of deformed crystal.

The displacement vector due to slip (Eq. 2.22) specifies the slip activity either via full dislocation slip or the partial slip.

\[ \tilde{\beta} = \overrightarrow{d_{def}} - \overrightarrow{d_{int}} \quad (2.22) \]

For atoms that are not slipped, such as atoms C and D, the dislocation vector is zero. The plastic deformation due to dislocations can be determined by using CSP or CAN parameter. The amount of strain due to partial or full dislocation glide can be evaluated by adding the strain from all atoms displaced by dislocation motion given by Eq. 2.23.

\[ \varepsilon^{dis} = \frac{1}{V} \sum_{i=1}^{N} \overrightarrow{A} \times (\overrightarrow{l} \cdot \overrightarrow{b_i}) \times \frac{1}{V} \sum_{i=1}^{N} \overrightarrow{A} \times (\overrightarrow{l} \cdot \overrightarrow{n}) \quad (2.23) \]

Where, \( \overrightarrow{n_i} \) is the unit normal of the slip plane for dislocation glide over atom i and \( \overrightarrow{b_i} \) is the Burgers vector associated with the dislocation and \( \overrightarrow{l} \) is the loading direction and A is
the unit area of atoms projected on the slip plane and \( V \) is the volume of the simulation box, and \( N \) is the total number of atoms that are slipped.

Another interesting tool to study the plastic deformation due to dislocations is using the Dislocation Extraction Algorithm (DXA), which is based on the construction of the Burgers circuit [74,75]. DXA analysis provides detailed information on the dislocation type, Burgers vector, dislocation character (edge, mixed or screw), and dislocation density. A typical image of dislocations from DXA analysis of Cu-Nb nanocomposites undergoing uniaxial compression is shown in Fig. 2.3.

![Figure 2.3 Dislocations inside the Cu layer under uniaxial compression of Cu-Nb nanocomposites at a strain of 0.8 analyzed using the DXA method.](image)

**2.4 Conclusion**

Molecular Dynamics modeling for analysis of microstructural evolution undergoing deformation has been presented. Fundamentals of numerical implementation of MD
simulations are explained in detail. Parameters such as ensembles used to describe the state of the system, boundary condition, and kind of interatomic potentials used in the study are presented. Many body potential based on EAM type describing the bonding of Cu and Nb atoms has been adopted. Construction of Cu-Nb nanocomposites with interfaces based on the accumulative roll bonding processing and physical vapor deposition was explained. Post-processing techniques to understand the atomistic deformation were described.
Chapter 3: Accumulative Roll Bonded Cu-Nb nanocomposites

3.1 Introduction

Accumulative roll bonding (ARB) has proven to be a promising severe plastic deformation (SPD) process to obtain ultra-fine-grained metals/alloys and multilayered composites. This process consists of an accumulation of large strains by rolling the stacks of sheets reduced to desired thickness.

ARB process was invented by Tsuji et al.[76], where a multi-stage operation such as cutting, stacking, rolling is employed to obtain bonding between the stacked sheets. Schematic diagram of Fig. 3.1. indicate the process of ARB in a flow chart, where two or more sheets are assembled and passed between the rolls to apply plastic deformation [77]; The accumulation of plastic strains produces a solid-state bonding. For instance, Fattahi et al. [78] fabricated composite filler metals of Tungsten inert gas welding, which resulted in a significantly improved yield strength of Al$_2$O$_3$/TiC/TiO$_2$ nanoparticle/Al composite. Conducting the ARB process at elevated temperatures can result in better interfacial bonding [79]. Heat treatment processes such as annealing have also been used to achieve strong metallurgical bonding between the stacked layers [80]. Processing parameters such as rolling reduction, rolling temperature, rolling speed, and rolling friction affect bonding between the two surfaces. One of the main theories proposed to explain the bonding mechanisms is a Film theory, which advocates that if two clean metal surfaces are stacked in close contact and deformed to a sufficiently large value may create a bonding. ARB fabricated Cu-Nb nanocomposites predominantly adopt the Kurdjumov–Sachs (KS) with \{112\} FCC Cu || \{112\} BCC Nb orientation at the
interface joining Cu and Nb [81]. These interfaces are faceted in nature, with a regular array of misfit dislocations to accommodate the mismatch between the habit planes of Cu and Nb. The construction of such an interface using computer modeling is explained in the section 3.3 of chapter 3.

Figure 3.1 Schematic process of accumulative roll bonding involving stacking, rolling, cutting [77].
3.2 Evolution of interface textures in Cu-Nb nanocomposites

The interface texture of Cu-Nb multilayered composites depends on the type of manufacturing route. The cubic structures of Cu and Nb result in a cube-on-cube crystal orientation at the interface.

During the severe plastic deformation of Cu and Nb layers using ARB, mechanically deformed interfaces arise. These interfaces predominantly adopt the KS with \{112\} FCC Cu || \{112\} BCC Nb misorientation relationship [23]. The high-resolution transmission electron microscopy (HRTEM) image of Fig. 3.2 indicate the above misorientation relationship. Furthermore, these interfaces are faceted in nature and contain misfit dislocations with both in-plane and out-of-plane Burgers vectors [82], which appear in the Cu layer. Interfaces play a predominant role in controlling the deformation mechanisms in MNCs because of their ability to block, transmit and provide nucleation

![Figure 3.2](image)

**Figure 3.2** (a) Kurdjumov–Sachs (KS) with \{112\} FCC Cu || \{112\} BCC Nb misorientation relationship. (b) Kurdjumov–Sachs (KS) with \{110\} FCC Cu || \{112\} BCC Nb misorientation relationship [82].
sites for dislocations.

Two important interface characteristics that affect the transmission are:

**Alignment of slip systems:** While the geometrically favorable slip systems of individual layers across the interface provide easy and efficient pathways for dislocation transmissions, discontinuous slip systems act as barriers [83].

**Interfacial shear strength:** Dislocations approaching the interfaces with low shear strength tend to get absorbed. Interfaces with high shear strength are less likely to shear and hence promote dislocation transmission [83].

### 3.3 Simulation Geometry

The molecular dynamics (MD) simulations of Cu-Nb multilayered composites (MC) were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) under embedded atom method potential [20]. The Ovito software [21] was utilized to visualize MD trajectory data after deformation under uniaxial tension and compression of strain rate (3×10^8 s⁻¹). The temperature of the system was controlled using a Nose-Hover thermostat.

The Cu-Nb interfaces under investigation were constructed in a bilayer fashion [10]. The bilayer consisted of {112} face-centered cubic (FCC) Cu connected to free surface of a {112} body-centered cubic (BCC) Nb. A total of 54-unit cells of Cu were stacked over a 76-unit cell of Nb to obtain a Cu-Nb bilayer of 8nm/8nm layer thickness. The Cu-Nb bilayer cross-section parallel to the interface is a rectangle with dimensions 4 nm by 7 nm. To ensure periodicity in the interface plane, the plain strain was applied to one of the adjoining layers. The shape and dimensions of the Cu-Nb layers were chosen such that
this strain is minimized. The relaxed structure of the Cu-Nb system with orientations referred from the KS interface with ARB processed samples is shown in Fig. 3.3. Due to crystal structure mismatch between Cu and Nb, misfit dislocations were observed extending into the Cu layer as indicated by the white circles and ellipses. Similar observations were also recorded in the molecular dynamics study by Kang et al. [22].

The discussion of the deformation behavior of Cu-Nb multilayered nanocomposites is divided majorly into three parts, namely, the compression response, the tension response, and the comparison between the two. The results are arranged describing the elastic, 

![Figure 3.3 Relaxed structure of FCC Cu<112>||BCC Nb<112> in the Kurdjumov–Sachs (KS) orientation relation. The model is under periodic boundary conditions (PBCs). Due to the crystal structure mismatch, the misfit dislocations were observed extending into the Cu layer as indicated by white circle and ellipse.](image-url)
yield, post-yield (hardening), and failure stages of deformation under the above types of loading.

3.4  Deformation behavior of ARB processed Cu-Nb nanocomposites

3.4.1 Under compression normal to interfaces:

Compression normal to the interface involves loading perpendicular to the FCC Cu \{112\} || BCC Nb \{112\} interface. Fig. 3.4 describes the compression stress-strain response of Cu-Nb nanocomposites upon loading normal to the interface. The elastic segment of the stress-strain curve is quantified by the elastic modulus. The Elastic Modulus of a composite under iso-stress loading mode (loading normal to interfaces) is described by Eq. (3.1).

\[
E_{iso-stress} = \frac{E_{Cu}E_{Nb}}{E_{Nb}V_{Cu} + E_{Cu}V_{Nb}} \tag{3.1}
\]

where, \(E_{Cu}\) is the Elastic Modulus of Cu \(<112>=145\) GPa \[84\] and \(E_{Nb}\) is the Elastic Modulus of Nb = 105 GPa. \(V_{Cu}\) and \(V_{Nb}\) are the volume fractions of Cu and Nb, respectively. The modulus values computed from MD simulations are consistent with the values computed from composite theory (Eq. 3.1) are reported in Table 1. The three-dimensional crystallographic orientation of ARB processed Cu-Nb system can be described by orientations Cu\{111\} and Nb \{110\} along X-axis, Cu \{110\} and Nb \{111\} along Y-axis and Cu \{112\} || BCC Nb \{112\} at the interface along Z-axis.

As shown in the stress-strain diagram of Fig. 3.4 (i) (purple color), the compressive stress linearly increases until the maximum stress of 10 GPa and strain of 0.06. Under compression normal to the interfaces, the plasticity commences when the stress reached
3.29 GPa as indicated by the point the ‘a’, in Fig. 3.4. (i) via the nucleation of dislocations at the interface into the Cu layer. The corresponding molecular dynamic trajectory of the point ‘a’ is as shown in Fig. 3.4. (ii) a. The atoms are color-coded according to the common neighbor analysis (CNA). The red atoms represent hexagonal close-packed stacking, green atoms represent face-centered cubic stacking, and the blue atoms represent the body-centered cubic structure. When the applied strain is around 2%, dislocation nucleates on (11̅1) plane at the interface and glides along the [11̅2] direction. These are identified as Shockley partials with a Burgers vector [112]/6, which leaves a stacking fault behind. The Shockley partial propagates towards the adjacent interface. As the deformation progresses, another Shockley partial dislocation of identical Burgers vector nucleates at the interface, as shown in Fig. 3.4. (ii)b. The two Shockley partials glide on parallel planes. The two stacking faults expand as the partial dislocations continue to glide, leading to nucleation of a twin of two atomic layer thickness as shown in Fig 3.4. (iii)c. Upon further deformation, the twin continues to grow along with the gliding of Shockley partials. At a strain of around 9.2% and stress of 9.8 GPa, dislocations transmit across the interface from Cu into Nb. Indeed, the transmission of dislocations across the interface is a dominant plastic deformation in a multilayered nanocomposite when the layer thickness of the composite phases was reduced below a few nanometers range. In addition, the slip transmission across the interface is ascribed to factors such as interface shear strength, the elastic mismatch, and differences in Burgers vectors. In the case of ARB processed Cu-Nb faceted interfaces as such in our study, the transmission of dislocation
across the interface is from Cu to Nb because Nb has a smaller Burgers vector as observed by Zhang et al. [85] in their study on shock compression of Cu Nb MNCs.

![Graph and Diagram](image)

**Figure 3.4** (i) The compression under iso-stress (ii) The MD trajectory snapshots taken at different strains indicating compression twins in the case of iso-stress condition.
3.4.2 Under compression parallel to interfaces:

The effect of loading parallel to the interfaces (iso-strain) on the mechanical response is as shown in Fig. 3.5. (i) (in Maue color). The crystallographic orientation corresponding to iso-strain loading is along Cu {111} || BCC Nb {110}. The iso-strain elastic Modulus of a composite is given by Eq. (3.2).

\[ E_{iso-strain} = E_{Nb}V_{Cu} + E_{Cu}V_{Nb} \]  \hspace{1cm} (3.2)

where, \( E_{Cu} \) is the Elastic Modulus of Cu <111> = 190 GPa [84] and \( E_{Nb} \) is the Elastic Modulus of Nb = 105 GPa. The resulting elastic Modulus under iso-stress and iso-strain are summarized in Table.1. The anisotropy in the elastic Modulus under compression loading parallel and normal to interface match well with the composite theory calculations (see table.1). The compressive stress-strain response under iso-strain loading is represented as shown by Maue color (circle data points) in Fig. 3.5. (i). The plastic activity begins with activation of Shockley partial dislocation on (11\bar{1}) plane and glides along [11\bar{2}] direction, leaving a stacking fault behind. The above observation is similar to that under loading normal to interfaces (see Fig. 3.5. (ii)c & d). However, unlike loading normal to interfaces, twinning does not occur when loading along parallel to the interfaces. The likelihood of slip or twinning depends on various factors such as stacking fault energy (SFE), crystallographic orientation, size, shape, loading mode, and strain rate. Upon compression along the direction parallel to the interface, <111> Cu and <110> Nb, plasticity is occurred by nucleation of leading Shockley partial immediately followed by trailing partial, thus constituting an extended dislocation. Compression parallel to Cu-Nb interfaces along <111>Cu and <110>Nb, the deformation occurs
completely by dislocation slip. We also observe multiple slip systems being activated in the Cu layer. This behavior is expected because of its FCC crystal structure and availability of multiple slip systems when compressed along <110> direction. Another important observation was the transmission of dislocation from Cu to Nb layer at a strain of 0.05. Dislocations transmit at lower strain and stress levels when the loading is parallel to interfaces along [111] Cu direction. This observation points towards the effect of loading direction on the interface resistance for dislocation transmission.

Figure 3.5 (i) The compression behavior of Cu-Nb MNCs under iso-strain loading (ii) The MD trajectory snapshots taken indicating deformation through slip in case of iso-strain condition.
3.4.3 Under tension normal to interfaces:

The elastic response of 8m-8nm Cu-Nb multilayered nanocomposites under tension normal to the interfaces is illustrated in Fig. 3.6. The stress-strain diagram in Fig. 3.6. (i) (in salmon color) describes the elastic region of the nanocomposites, where the stress component along Z-direction increases linearly with strain for up to 4.6 GPa. During this deformation stage, the preexisting dislocations of edge type extend from the interface.
into the Cu layer bow in response to the applied stress, as shown in Fig. 3.6.(ii).a. The traditional ‘elastic string’ theory approximation regards the dislocation line as having a tension of the order $0.5\mu b^2$, where $\mu$ is a shear modulus, and $b$ is the magnitude of Burgers vector. The stress required to make the dislocation unstable is given by $\mu b/L$, where $L$ is the length of the dislocation line, and the shape of the critical segment is a semicircle.

<table>
<thead>
<tr>
<th>Mode of loading</th>
<th>Elastic Modulus from MD simulations (GPa)</th>
<th>Elastic Modulus from composite theory (GPa)</th>
<th>Yield (GPa)</th>
<th>Maximum stress (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iso-stress</td>
<td>121.8</td>
<td>125</td>
<td>4.6</td>
<td>10</td>
</tr>
<tr>
<td>Iso-strain</td>
<td>147.5</td>
<td>153</td>
<td>4.56</td>
<td>8.5</td>
</tr>
</tbody>
</table>

*Table 1. Comparison of elastic modulus, yield and maximum stress between iso-stress and iso-strain loading conditions.*

The maximum radius up to which the bowing occurs is equal to 7nm in our case for the applied stress of 2.7 GPa.

The elastic stress fields of bowed dislocations from adjacent interfaces interact and repel because of their opposite Burgers vector gliding on different planes, as shown in Fig. 3.6(ii).a. Upon further increase in stress, the slip initiates on $(1\bar{1}1)$ plane along $\langle 110 \rangle$ direction in Cu layer at a stress of 4.6 GPa, which is identified as the yield point. Post-yielding behavior consists of series of slip activations further followed by forest hardening. The dislocations of type $\langle 110 \rangle$ dissociate into Shockley partials of type $\langle 112 \rangle$. The hardening was attributed to the interaction between Shockley partials and other $\langle 110 \rangle$ types of dislocations. Dislocations of $\langle 112 \rangle$ type gliding on intersecting $(111)$ planes
form a series of obstacles known as ‘Lomer-Cottrell’ locks, of <110> stair-rod type of dislocation as shown in Fig. 3.6 (ii)b. These Lomer-Cottrell locks are sessile dislocation and hence lead to stress concentration. Furthermore, this stress concentration point at the interface leads to the formation of a micro-void type of structure, as shown in Fig. 3.6(ii) c. They are leading to failure at the interface. We point out that, while the above discussions were specifically in the Cu layer of the nanocomposites, the dislocation activity in Nb could only be seen at very high strain values.

**Figure 3.7** (i) The tensile behavior of Cu-Nb MNCs under iso-strain loading (ii) The MD trajectory snapshots taken indicating deformation slip and nucleation of twin at the interface via emission of Shockley partials.
3.4.4 Under tension parallel to interfaces:

Under tension parallel to Cu-Nb interfaces, the straining happens along the Cu<111>∥Nb<110> as shown in Fig. 3.7 (i). The elastic response is similar to that of tension normal to the interfaces. However, a study by P. Rohith et al. [86] indicates that the deformation mechanisms in Cu nanowires depend on crystallography. Their deformability maps show that, while the tension along <111> direction of Cu nanowire leads to twinning, tension along <001>Cu leads to slip-assisted plastic mechanisms. Similar deformation mechanisms (twining) were observed under tension along Cu<111>∥Nb<110> MNCs. However, as explained under the section, tension normal to interfaces, that is, tension along Cu <112>∥Nb<112>, slip instead of twinning was observed (see Fig. 3.7(ii) d & e). The above observation indicates the effect of Cu-Nb interfaces on the deformation mechanisms. It is noteworthy to mention that the hardening rate for tension in parallel orientation is significantly higher than that of normal orientation (see Fig. 3.6 (i)).

3.5 Conclusion

One of the key features responsible for initiating plasticity in MNCs is dislocation nucleation at the metal-metal interface. This letter investigated the effect of loading direction and crystallography on the mechanical response of MNCs. Using molecular dynamics simulations, we described the elastic, yield, hardening stages of Cu-Nb MNCs with ARB processed interface structures. This work also shows that crystallography and
loading direction indeed affect the atomic-scale deformation mechanisms in Cu-Nb MNCs. In addition, the manuscript provides tension-compression asymmetry present in the MNCs. While the compression behavior under iso-stress conditions showed deformation through partial slip leading to twinning, compression parallel (iso-strain) to interfaces indicate only slip mechanisms. On the contrary, the behavior changes to slip for tension under iso-stress conditions, and partial slip occurs for tension under iso-strain conditions. When the above deformations occur predominantly in the Cu layer, plasticity in the Nb layer occurs via either dislocation transmission or nucleation at only very high strains.
Chapter 4: Cu-Nb multilayered Nanocomposites fabricated by Physical Vapor Deposition

4.1 Introduction

Physical vapor deposition (PVD) via magnetron sputtering is a bottom-up thin film deposition technique where the required metal/alloy combination is grown on the solid surface, as shown in Fig. 4.1. Thin films deposited by the process of atomization or vaporization usually have microstructures with layers of thickness varying from atomic to micron-scale [87-90].

Joining of nanostructured metals by the process of physical vapor deposition (PVD) such as Cu/Nb [91], Cu/Ni [92], Nb/NbC [93], Cu/W [94], and Mg/Nb [95] involves two different kinds of sources are mounted, and thin alternate layers are deposited to obtain the nanolayered architecture (a few microns thick). Magnetron sputtering is beneficial in

Figure 4.1 Schematic of PVD process via evaporation [88]
fabricating nanolaminates due to low deposition temperature, control of coating composition, thickness, and better adhesion between the layers [96]. A multilayered bimetal composite with individual layer thickness ranging from a few nanometers to a few tens of nanometers can be fabricated via PVD deposition. Furthermore, the interface between the layers can be uniform and depends on the deposition epitaxy. The type of epitaxy that is the growth of crystal orientation and the interface characteristics are driven by the thermodynamics of the deposition. In particular, the main criterion governing the interface characteristics is defined by the minimization of interfacial energy associated with the growth of the layers under a given set of conditions such as temperature, pressure, deposition rate, and the substrate [97].

One of the drawbacks of magnetron sputtering is the requirement of a high vacuum system. This factor makes the deposition process expensive and limits the total thickness

Figure 4.2 HRTEM image of: (a) K-S interface (111) FCC || (110) BCC in Cu-Nb nanocomposite (b) N-W interface with (111) FCC || (110) BCC in Cu-Nb nanocomposite [97].
of the deposited film. The deposition parameters such as temperature, deposition rate, alternate deposited layers may vary the microstructure properties of the nanolaminates. The PVD deposition of Cu-Nb yields a specific crystallographic orientation at the interface between Cu and Nb layers. Interface orientation relationships such as Kurdjumov–Sachs (K-S) or Nishiyama–Wasserman (NW) orientation relationship joined at the Cu \{111\} FCC \| Nb \{110\} BCC interface planes as shown in [97] Fig. 4.2. The microstructure of the PVD deposited nanocomposites influences the mechanical properties. The atomic-scale investigation of the Cu-Nb interface structure revealed that they are atomically sharp, ordered with a well-defined misfit dislocation pattern, and atomically flat [97]. The construction of such an interface showing those atomic-scale features is shown in Fig. 4.3 and explained in section 2 of Chapter 4.

4.2 Analysis of atomic interface structure

Multilayered nanocomposites (MNCs) with nanolayers are fabricated via physical vapor deposition (PVD). Previous atomistic simulations and electron microscopy experiments on PVD deposited Cu-Nb MNCs have shown to have FCC Cu \{111\} \| BCC Nb \{110\} interface orientation. The Cu-Nb MNCs in this study were fabricated in a bilayer fashion by joining FCC Cu \{111\} to BCC Nb \{110\}. The volume fractions of Cu and Nb are equal with an individual layer thickness of 5nm. Periodic boundary conditions were applied to all three dimensions to ensure the connectivity between the layers forming a multilayered structure and to reduce the number of atoms in the system. The above structure was produced using Atomsk software. MD simulations were performed using a
Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) under embedded atom method potential [98]. The challenging aspect of MD simulations is the inherent limit on a time scale set by the vibrational frequencies of the atom.

This limitation restricts the simulation from being simulated for longer times, and only a few nanoseconds can be simulated. Hence, a very high strain rate has to be applied to achieve plastic deformation. The Ovito software [99] was utilized to visualize MD trajectory data after deformation under uniaxial tension and compression of strain rate (3×10⁹s⁻¹). The temperature of the system was controlled using Nose- Hover thermostat. The system was equilibrated first by applying energy minimization at 0K until the maximum force on any atom was smaller than 1×10⁻¹⁰ N. The relaxed structure of the Cu-Nb system with orientations as referred from the KS interface with PVD processed samples are as shown in Fig. 4.3. The relaxed structure in Fig. 4.3 indicates that the interface is

![Figure 4.3 Relaxed structure of PVD Cu-Nb interface which is atomically sharp and regular pattern of dislocations.](image-url)
ordered and atomically flat, unlike the faceted structure in the case of Cu-Nb MNCs with ARB interfaces (See Fig. 3.3). A regular array of misfit dislocations was observed in the relaxed structure to accommodate the lattice mismatch between Cu and Nb layers (marked by yellow circles in Fig. 4.3).

The discussion of the deformation behavior of Cu-Nb multilayered nanocomposites is divided majorly into three parts, namely, the compression response, the tension response, and the comparison between the two. The results are arranged describing the elastic, yield, post-yield (hardening), and failure stages of deformation under the above types of loading.

4.3 Interface Formation Energy of PVD Cu-Nb MNCs
The thermodynamic factor that governs the stability and epitaxy of the bi-metal interfaces depends on the minimization of interfacial energy. The interfacial energy of an interface can be calculated using Eq. (4.1).

\[ \gamma_{i}^{Cu-Nb} = \frac{1}{A} (E_{Bl} - E_{coh}^{Cu}N_{Cu} - E_{coh}^{Nb}N_{Nb}) - \gamma_{fs}^{Cu} - \gamma_{fs}^{Nb} \]  

Where, \( \gamma_{i}^{Cu-Nb} \) is the interfacial energy of Cu-Nb bi-metal interface, \( E_{Bl} \) is the potential energy of the bilayer, \( A \) is the area of the interface and \( E_{coh}^{Cu} \) and \( E_{coh}^{Nb} \) are the cohesive energies of the Cu and Nb, respectively. \( \gamma_{fs}^{Cu} \) and \( \gamma_{fs}^{Nb} \) are the free surface energies of Cu and Nb, respectively. Cohesive energy is the energy required to separate an atom from a crystalline solid. \( E_{coh}^{Cu} = 3.52 \text{ eV/atom} \) [100] and \( E_{coh}^{Nb} = 7.57 \text{ eV/atom} \) [101]. The interfacial energy of the Cu-Nb system with PVD interfaces was around 560 mJ/m².
4.4 Deformation behavior of PVD fabricated Cu-Nb nanocomposites

4.4.1 Under compression normal to interfaces (Iso-Stress Loading):

The compressive response of FCC Cu [111] || BCC Nb [110] interface oriented normal to the direction of loading is depicted in Fig. 4.4. The corresponding stress-strain response of the Cu-Nb MNCs under iso-stress conditions is as shown in Fig. 4.4. (i). At a strain of 0.003 represented by point ‘a’ in Fig. 4.4. (i), stacking faults parallel to the

![Graph showing stress-strain response](image)

**Figure 4.4** The compression stress-strain under iso-stress (pine green)). (ii)

The MD trajectory snapshots taken at different strains indicating compression twins in the case of iso-stress condition.
interface plane were observed in the Cu layer. The atoms are color-coded according to
the common neighbor analysis (CNA). The red atoms represent hexagonal close-packed
(HCP) stacking, green atoms represent face-centered cubic (FCC) stacking, and the blue
atoms represent the body-centered cubic structure (BCC), the white atoms represent
uncoordinated atoms which neither belong to FCC, BCC, or HCP.

The plastic activity begins in the interior of the Cu layer with the formation of stacking
defects (See Fig. 4.4. (ii)a). With an increase in strain, the Shockley partials deform into
twins, as shown in the MD trajectory of Fig. 4.4 (ii)b. Several past experimental and
atomistic studies of PVD deposited Cu-Nb interfaces under a variety of stress states,
including rolling [102], in plane-tension [103], and micro compression perpendicular to
the interfaces indicated either a little or no evidence of twinning [104]. In our work,
twinning was observed in the PVD deposited Cu-Nb MNCs under compression in the
iso-stress condition. The observed twinning was not originated at the interface; instead,
the twinning was believed to be originated through the climbing of stacking faults in the
Cu layer at a distance of 8d₀ (see Fig. 4.4 (ii).b) from one of the interfaces, where d₀ is the
interplanar distance of [111] Cu. This type of twinning was observed in a molecular
dynamics study of bending of Cu nanowires [105]. There is drop-in stress from point ‘b’
to ‘c,’ and the corresponding MD trajectory of point ‘c’ is as shown in Fig. 4.4. (ii)c, it
can be seen that a dislocation nucleates at the interface into the Nb layer and also seen is
the dislocation from the interface into the Cu layer (See Cu Layer of Fig. 4.4 (ii)c. This
dislocation in the Cu layer intersects with the stacking fault and twin with subsequent
straining, as shown in Fig. 4.4 (ii)d and Fig. 4.4 (ii)e. The interface is seen to act as a
dislocation nucleation source generating a plethora of Shockley partials into Cu and Nb layers. The Shockley partials in the Cu layer interact with stacking faults, twin boundaries, and each other. These dislocations transmit across the stacking faults and twin boundaries and deposit at an adjacent interface. This behavior is seemed to be the characteristic of computer simulations with small layer thicknesses and very high strain rates.

4.4.2 Under compression parallel to interfaces (Iso-Strain Loading):

![Graph and images showing stress-strain behavior under iso-strain loading with snapshots indicating deformation through slip.](image)

**Figure 4.5** The compression stress-strain under iso-strain behavior (yellow triangle) (ii) The MD trajectory snapshots taken at different strains indicating deformation through slip in case of iso-strain condition.
The effect of loading parallel to the interfaces (iso-strain) on the mechanical response is as shown in Fig. 4.4.1. The crystallographic orientation corresponding to iso-strain loading is along FCC Cu \{211\} || BCC Nb \{112\}. The compressive stress-strain response under iso-strain loading is represented as shown by yellow color (triangle data points) in Fig. 4.5 (i). The plastic activity begins first in the Cu layer by the formation of stacking faults, which are arranged parallel to the interface as shown in Fig. 4.5 (ii)f, similar to that of iso-stress loading. The point ‘g’ on the stress-strain plot in Fig. 4.5. i. corresponds to nucleation of Shockley partial dislocations at the interface and emit into the Cu layer (see 4.5 (ii)g). These Shockley partials intersect with previously existed faults to form a different set of stacking faults which are oriented perpendicular to the interface. Plastic activity in Nb begins at a much later stage when the strain value is 0.082, where dislocation activity in the Nb layer can be seen (See Fig. 4.4(ii)h). The point ‘h’ on the stress-strain plot corresponds to a stress value of around 12 GPa. Further increase in strain results in dislocation nucleation and propagation from the interface into the Nb layer with simultaneous deformation occurring in the Cu layer resulting in co-deformation of Cu and Nb.

4.4.3 Under tension normal to interfaces (iso-stress condition):

The elastic response of 5m-5nm Cu-Nb multilayered nanocomposites under tension normal to the interfaces is illustrated in Fig. 4.6 (i). The plastic deformation in tension involves the formation of stacking faults, as shown in Fig. 4.6 (ii)a. and resulting in twinning with further deformation (see Fig. 4.6 (ii)b.). Although the formation of stacking faults and
twinning is similar to that of compression behavior, the arrangement and the role of these structural features on the further deformation is quite different in the case of tensile loading. At point ‘e’ on the stress-strain plot corresponds to the stress of 8.8 GPa, a Shockley partial dislocation originated at the Cu-Nb interface and glides along the \{111\} plane of Cu. The passage of dislocation across the (111)\textsubscript{T} twin boundary is illustrated in Fig. 4.6 (ii) d & e. The point ‘d’ on the stress-strain plot in Fig. 4.5. i indicate dislocation blockage by the first twin interface TB\textsubscript{1}. Further, an increase in loading involves dislocation transmission

**Figure 4.6** The comparison of tension stress-strain curves under iso-stress (Red)

(ii) The MD trajectory snapshots taken at different strains indicating deformation via slip and twinning under iso-stress condition
across the 4-layer twin, Fig. 4.6 (ii)h. Although the Shockley partial emitted from the interface into the Cu layer glides on \(\{111\}\) plane, after traversing the TB\(_1\), its slip configuration suggests that it may be passing through the twin by cross-slippping onto the unusual \((100)_{T}\) plane as marked by yellow lines in Fig. 4.6(ii)g. The two stress peaks correspond to points ‘f’ and ‘g’ on the stress-strain plot of Fig. 4.6 (i). are corroborated to dislocation transmission across TB\(_1\) and TB\(_2\), respectively. This dislocation-twin interaction has been observed in various nanocrystalline FCC metals studied using MD [106], [107]. The contributing factors for this unusual dislocation-twin interaction are the high strain rate deformation during the MD simulations, where an incoming dislocation may not be allowed to have enough time to adapt to a \(\{111\}\) slip plane but rather choose \(\{100\}\) plane as it is oriented in a favorable geometry with respect to the twin boundary \(\{111\}_{T}\). In addition, loading along the <111> direction gives rise to high Schmidt factor on \(\{100\}\) planes. Further deformation induces dislocation nucleation on the twin step, which glides along the \(\{1-11\}\) plane of FCC Cu inclined at 70° with TB\(_1\) at a stress of 10 GPa. With further increase in stress, a stacking fault tetrahedron is formed inside the twin lamella, which leads to concentration and cracking, as shown in Fig. 4.6 (ii)g. It is very important to note that the crack initiation and propagation in the case of PVD Cu-Nb MNCs occur in one of the bi-layers, that is, the Cu layer, unlike cracking at the interface in the case of ARB Cu-Nb MNCs (See Fig. 3.5 (ii)d). This observation indicates that the PVD interfaces are more stable towards the deformation as compared to the ARB interfaces. The difference in the stability of interfaces could be because of the difference in the interface formation energies of the Cu-Nb nanocomposites. The lower the interface
formation energy, the stronger is their stability. The interfaces of type KS {111} Cu || {110} Nb from PVD deposition have an interface formation energy of 560 mJ/m² which is lower than the ARB KS interface of type of {112} Cu || {112} Nb with 870 mJ/m².

4.4.4 Under tension parallel to interfaces (iso-strain condition):

Figure 4.7 The comparison of tension stress-strain curves under iso-strain loading condition (blue) (ii) The MD trajectory snapshots taken at different strains indicating deformation via slip, twinning, stacking fault formation and transmission of dislocation from Cu to Nb across the interface.
Under tension parallel to Cu-Nb interfaces, the straining happens along Cu<-211>‖Nb<-112>. The plasticity was first observed in the Cu layer with the formation of stacking faults similar to iso-stress conditions.

However, the stress-strain of iso-strain response as shown in Fig. 4.7(i) represented in the blue curve varies significantly from that of tension in iso-stress conditions. With the increase in stress, a dislocation is emitted from the interface, which interacts with the stacking fault, as shown in Fig. 4.7(ii). Further deformation results in the annihilation of dislocations resulting in dislocation-free crystals with stacking faults. The next plastic event corresponds to peak point ‘L’ on the stress-strain diagram of Fig. 4.7(i). Results in dislocation emission from the interface into the Nb layer on (101) plane (See Fig. 4.7(ii) L). Further plastic activity occurs via co-deformation of both Cu and Nb.
Chapter 5: Conclusions

In this thesis, atomic-scale deformation mechanisms of Cu-Nb nanocomposites with interface orientations fabricated via accumulative roll bonding (ARB) and physical vapor deposition (PVD) processed are studied using Molecular Dynamics simulations. The effect of crystallography on the mechanical deformation behavior of multilayered nanocomposites (MNCs) is considered in detail. The following conclusions can be drawn from this thesis:

1. Construction and characterization of ARB processed Cu-Nb nanocomposite:
   Using the Atoms software, we constructed an 8nm-8nm Cu-Nb nanocomposite by joining the {112} Cu FCC $\parallel$ {112} Nb BCC. The sample is then relaxed using LAMMPS software to achieve the required energy minimization.

2. Mechanical characterization of ARB processed Cu-Nb MNCs: Uniaxial compression and tension tests were carried out using LAMMPS under iso-stress, and iso-strain conditions were carried out at room temperature and $10^8$ S$^{-1}$ strain rates. While the compression behavior under iso-stress conditions showed deformation through partial slip leading to twinning, compression parallel (iso-strain) to interfaces indicate only slip mechanisms. On the contrary, the behavior changes to slip for tension under iso-stress conditions, and partial slip occurs for tension under iso-strain conditions. When the above deformations occur predominantly in the Cu layer, plasticity in the Nb layer occurs via either dislocation transmission or nucleation at only very high strains.
3. Construction and characterization of PVD processed Cu-Nb nanocomposite: In the case of Cu-Nb nanocomposites with PVD interfaces, 5nm-5nm Cu-Nb nanocomposites were constructed by joining pure {111} Cu with the {110} pure Nb. The structure is relaxed using LAMMPS, and the interfacial characterization showed atomically sharp interfaces, which are flat and contained patterned misfit dislocations.

4. Mechanical Characterization of PVD processed Cu-Nb nanocomposites: The Effect of the interface, crystallographic orientation on the tension, and compression behavior of Cu-Nb nanocomposites indicated that dislocation nucleate at the interface and interact with the twin boundary or stacking fault under both tension and compression mode of loading. Furthermore, the formation of stacking fault tetrahedron was observed under tension. For the case of tension normal to the interfaces, cracks originate in the Cu layer without any deformation in the Nb layer. Whereas under compression and tension under iso-strain loading, Cu and Nb were observed to be co-deforming without any sign of cracks for a large strain value.

5. Our thesis outlined the effect of loading mode (Tension vs. Compression), crystallography, and mode of loading (Iso-strain and Iso-stress) on the mechanical response of Cu-Nb nanocomposites with two unique interface orientations. Furthermore, atomic-scale mechanisms including slip, twinning, and interaction between dislocation-twin and dislocation-interface in the MNCS were detailed.
Appendix

Code to generate the bi-metal Cu-Nb multilayered structure using Atomsk

--create fcc 3.615 Cu orient [-211] [0-11] [111] -orthocell -duplicate 13 15 8

cu_sc_b.cfg

# Generates Cu single crystal with FCC crystal structure having a lattice constant of
# 3.615 Å and orientation of [-211] along X-direction and [0-11] along Y-direction and
# [111] along Z-direction of the simulation box.

--create bcc 3.3 Nb orient [-112] [1-11] [110] -orthocell -duplicate 7 12 12 nb_sc_c1.cfg

# Generates Nb single crystal with BCC crystal structure having a lattice constant of 3.3
# Å and orientation of [-112] along X-direction and [1-11] along Y-direction and [110]
# along Z-direction of the simulation box.

cu_nb_shift.cfg -select Nb -def X -0.10245194 0 -def Y -0.0 0 -select Cu -def X 0 0 0 0 0 0

cu_nb_b.cfg -select Cu -def X 0.228457527 0 -def Y 0.118025186 0 -select Nb -def X 0.2284575270 -select Nb -shift 0 0 0.12288 cu_nb_bf.cfg

# Application of deformation strains to maintain the periodicity at the Cu-Nb interface.

--merge z 2 cu_sc_b1.cfg nb_sc_b1.cfg cu_nb_single_a1.cfg

# The merge command joins the single crystal Cu and Nb at the interface along the Z-
# direction to produce the K-S {111} Cu and {110} Nb.
Input file for Deformation of bi-layered crystal, Copper, and Niobium

# Input file for bi-layered crystal, Copper and Niobium
# ------------------------- INITIALIZAION --------------------------
clear
units metal
dimension 3
boundary p p p
atom_style atomic
# ------------------------- ATOM DEFINITION -----------------------
read_data cu_nb_test.lmp
# ------------------------- FORCE FIELDS -------------------------
pair_style eam/alloy
pair_coeff * * CuNb_eam1.eam.alloy Cu Nb
#---------------------Settings---------------------------------
compute pot all pe
compute csym all centro/atom fcc
compute eng all pe/atom
compute eatoms all reduce sum c_eng
compute 1 all stress/atom NULL
compute force all group/group all
#compute 1 all fep 298 pair eam/alloy volume yes

#---------------------------Run Minimization---------------------
reset_timestep 0
timestep 0.005
fix 1 all box/relax iso 0.0 vmax 0.001
thermo 10
min_style cg
minimize 0 1e-100 5000 5000
thermo_style custom step temp pe etotal press vol
thermo_style custom step pe press c_eatoms fmax
unfix 1
run 1000
#variable natoms equal "count(all)"
#variable totenergy equal "pe"
#variable length equal "lx"
#variable ecoh equal "v_totenergy/v_natoms"
#print "Total energy (eV) = ${totenergy}"
#print "Number of atoms = ${natoms}"
#print "Lattice constant (Angstoms) = ${length}"
#print "cohesive = ${ecoh}"
#
# -------- Equilibration ---------------------------------------------
reset_timestep 0
timestep 0.005
velocity all create 0 12345
fix 3 all npt temp 10 10 0.5 iso 0 0 5 drag 1
thermo
thermo_style custom step press vol lx ly lz temp etotal
# RUN AT LEAST 10000 timesteps
run 4000
variable tmp equal "lz"
variable lo equal ${tmp}
#----------------Deformation-----------------------------------

undump 1
unfix 3
reset_timestep 0
fix 1 all npt temp 600 600 0.05 x 0 0 0.5 y 0 0 0.5
#fix 4 all ave/time 1 100 100 c_1[1] c_1[2] c_1[3]
#fix 5 all ave/time 1 100 100 v_Lx v_Ly v_Lz v_Vol
variable srate equal 1.0e9
variable srate1 equal "v_srate / 1.0e12"
fix 4 all deform 1 z erate ${srate1} units box remap x
variable strain equal (lz-v_lo)/v_lo
variable p2 equal "-pxx/10000"
variable p3 equal "-pyy/10000"
variable p4 equal "-pzz/10000"
thermo 100
thermo_style custom step temp press etotal v_p4 v_strain
run 25000
print "All done"
References


