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Tensile and Flexural Deformation of Nickel Nanowires via Molecular Dynamics Simulations

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1. Introduction

Metallic nanowires show great potential for applications in minimization of electronic devices due to their extraordinary mechanical strength and electrical properties. Their desirable property characteristics with the smallest dimensions for efficient transport of electrons show potential for use as interconnects and critical devices in nanoelectronics and nano-optoelectronics (Chen, et al., 2006). These metallic nanowires also show potential for applications in electronic packaging, nanoelectronic and nano mechanical devices. A significant issue in the application of these metallic nanowires is their structural strength and stability under mechanical and thermal loading conditions. The deformation behavior of these nanowires under different mechanical loads (for e.g., tensile, bending) is poorly known. Experimental investigations of these behaviors are impractical due to their size and the complications of applying these loading conditions via nano load cells within high resolution microscope systems. Computational techniques based on molecular dynamics (MD) simulations of the representative atomistic configuration of the metallic nanowires provide an effective means of understanding the mechanical deformation behavior of these nanowires.

In this chapter, we discuss the tensile and flexural dynamic deformation behavior of the Nickel (Ni) nanowires due to tensile loading and flexural bending via molecular dynamics simulations. The tensile and flexural deformation behaviors based on the atomistic model configurations of Nickel nanowires are analyzed. The stress-strain constitutive behavior, tensile strength and the Young's modulus for various Ni nanowire configurations are investigated and presented. The natural frequency of the flexural deformation of these nanowires via molecular dynamics simulations is obtained and analyzed. The simulation of the deformation behavior in metallic nanowires modeled as atomistic systems at finite temperatures is a dynamic process and is conducted using classical molecular dynamics.

Focusing on the mechanical behavior of nanowires, it is known that the properties of material configurations at nanometer dimensions can be rather different from those of the bulk material. In the past decades, the rapid progress of miniaturization of electronic devices and nanoscale measurement systems has aroused an interest in nanometer scale materials such as nanowires (Ju, 2004) (Liang, 2003) (Park, 2005) (Silva et. al., 2004), (Silva,

2004) and nanotubes (Liew et. al., 2004). These are not only known for their applications in nanometer scale integrated circuits but also for nanoscale tips of scanning tunneling microscope (STM) (Young, 1966) and atomic force microscope (AFM) (Binnig et.al., 1986). This chapter investigates the tensile and flexural deformation of Nickel (Ni) nanowires using the classical molecular dynamics (Frenkel & Smit, 2001) (Haile, 1997) (Plimpton, 1995), (Rapaport, 1997) (Schlick, 2002) simulation method. Molecular dynamics simulations provide a means to predict mechanical behavior of nano material systems. Experimental techniques for such mechanical behavior of the nano dimensional nanowire configurations, as discussed in this chapter are not only practical but are also difficult.

Prior work in the literature exists on the deformation of the Copper and Gold nanowires (Chang & Fang, 2003) (Ikeda et. al., 1999) (Ju et. al., 2004) (Liang & Zhou, 2003) (Liew et. al., 2003) (Park & Zimmerman, 2005) (Silva et. al., 2004) (Silva, 2004) via molecular dynamics (MD) methods. In this chapter, a nanowire configuration formed from the single crystals of Nickel in the <001> (longitudinal), <100> and <010> (transverse) directions is employed. In particular, this chapter focuses on the mechanical properties of Nickel nanowires by means of molecular dynamics methods. The yielding and the fracture mechanisms (e.g., stress-strain relation of Ni nanowires, which are elongated by a tensile deformation are investigated. The effects of strain-rate, specimen size and ensemble temperature (Chang & Fang, 2003) (Cheung & Yip, 1994) on the tensile deformation behavior are addressed. Most of the current literature is focused on the tensile deformation of nanowire configurations of different materials with very limited and non-existent work on their bending deformation behavior. In addition to this tensile deformation, this chapter also focuses on the flexural deformation of the Nickel nanowire beams under flexural bending conditions via molecular dynamics modeling and simulations.

This chapter is organized as follows. Brief discussions on the theoretical basis of molecular dynamics (MD) simulation methods which in essence are numerically similar to the solution of the multi-body dynamics problems in mechanics are presented. This is followed by a brief discussion on the computation of nano level stresses from the atomic displacement and velocity fields in such MD simulations. These numerical methodologies briefly described in this chapter form the basis of the general purpose molecular dynamics solver (LAMMPS: Large-Scale Atomic/Molecular Massively Parallel Simulator) from Sandia National Laboratory (Plimpton, 2005). The force field interactions between the Nickel atoms are modeled based on the embedded atom potential (EAM). This is followed by the discussions on the analysis of the tensile and flexural bending deformation behavior of Nickel nanowires under various boundary, loading and temperature conditions.

2. Overview of Molecular Dynamics Simulations

Molecular dynamics techniques are generally employed in the simulations of atomistic or molecular level systems. The solution approaches are similar to multi-body problems of mechanics. Computationally, a MD simulation consists of step-by-step numerical solution of the classical Newton equations of motion. The general form of the equations of motion used in MD simulations is given by

$$F_i \equiv -\nabla_i \Pi(X) \equiv -\frac{\partial \Pi(X)}{\partial X_i} = m_i \frac{d^2 X_i}{dt^2} \equiv m_i \frac{dv_i}{dt} \equiv m_i a_i \qquad (1)$$

.

In this chapter N is the total number of atoms, Π is the potential energy function, and X denotes the positions of atoms; m_i, v_i, and a_i are the mass, velocity and acceleration of atom i. Any molecular level system can be completely formulated by the positions X and velocity V (or momentum P) of atoms. The above equation is similar to the Newton equations of motion employed in continuum mechanics but applied at the atom level. The dynamic behavior of the time-dependent atom motion is computed using an integrator such as the Verlet integrator (Cheung & Yip, 1994) to calculate the trajectories of the atoms. The time-scale involved in the MD simulations is of the order of O (10^{-12} – 10^{-15} sec) and the length-scale is of order O (10^{-10} – 10^{-7} m). Figure 1 shows the general solution flow of the molecular dynamics simulations.

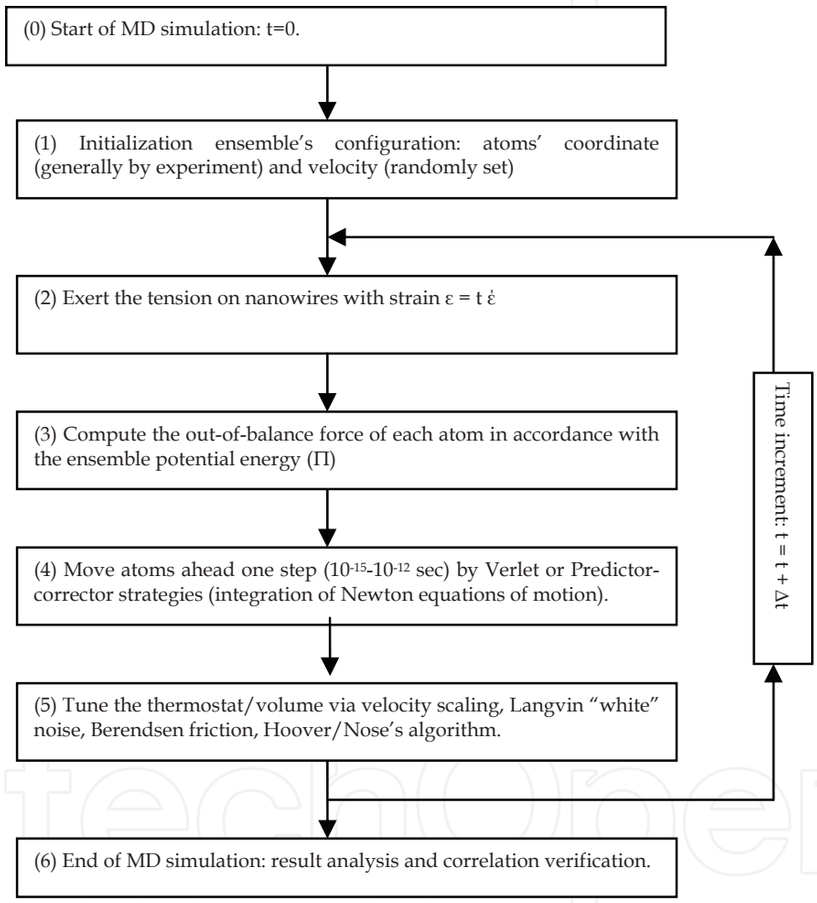


Fig. 1. Solution Flow of Molecular Dynamics Simulation

As illustrated in Figure 1, the numerical solution of Newton's equations of motion (Eq. 1) involved in the MD simulations consists of the following steps:

(1) An initial configuration (the location coordinates and velocity of atoms at time *t=0*). The initial coordinates of the atoms are generally obtained from experiments (Plimpton, 2005). In this work, the atoms of Nickel nanowires are initially configured according to the structure of Nickel crystal (FCC with lattice constant of ɔ=3.52Å) (Plimpton, 2005). The initial velocity of atoms is usually determined from a random distribution such that the molecular system has a zero initial momentum, as defined by Eq. 2.

$$P = \sum_{i=1}^{N} P_i = \sum_{i=1}^{N} m_i v_i = 0 \quad (2)$$

The velocities of atoms are also chosen randomly using Maxwell-Boltzmann and Gaussian distribution. For a given temperature T, the probability of an atom at velocity v is given by (Frenkel & Smit, 2001) (Haile, 1997) (Schlick, 2002)

$$\varphi(v_i) = \left(\frac{m_i}{2\pi k_B T} \right)^{1/2} \exp\left(-\frac{1}{2} \frac{m_i v_i^2}{k_B T} \right), \quad (3)$$

where k_B is Boltzmann's constant and T is absolute temperature. One of the difficulties in molecular dynamics simulation is calculating the temperature of the system, because temperature is a statistical quantity. However, if there are a large enough number of atoms, a statistical average temperature can be estimated from the *instantaneous temperature* (Frenkel & Smit, 2001) (Haile, 1997) (Schlick, 2002), which can be found from the kinetic energy of the system. This instantaneous kinetic temperature is given by

$$T = \frac{1}{3Nk_B} \sum_{i=1}^{N} \frac{P_i^2}{m_i} \quad (4)$$

This instantaneous kinetic temperature is an indication of the mechanical activity at the atomistic level. This temperature is employed in the simulation studies discussed in this chapter to understand the effect of temperature on the tensile deformation presented in a later section behavior of Nickel nanowires.

(2) Apply an external load/displacement/strain to the initial configuration. In this work, an external axial strain $\varepsilon=\dot{\varepsilon}t$ where $\dot{\varepsilon}$ is a constant strain-rate has been used for the tensile deformation and an external bending loading force is used for the flexural deformation.

(3) The deformation of the system under the action of an external force is computed using the potential energy function. Commonly used potential energy functions are empirical potentials, semi-empirical potentials, and ab-initio (first principles) potentials (Frankel & Smit, 2001) (Haile, 1997). Only empirical potentials are applicable for practical large-scale problems. Embedded atom method (EAM) (Frankel & Smit, 2001) (Haile, 1997) (Plimpton, 2005) (Schlick, 2002) is one such empirical potential that provides a precise and efficient description for metals and metal alloys. This potential is used in this study.

(4) The dynamical behavior of the atomistic system is computed using the potential Π and its gradient $\Delta\Pi$. The time integration gives a snapshot of the atomic configuration (called trajectory) that changes at each discrete time level. No analytical method is applicable for the solution of dynamic system (Eq.1). Commonly used numerical techniques include Verlet, leap-frog, velocity-corrected Verlet, Beeman and predictor-corrector methods (Frankel & Smit, 2001) (Haile, 1997) (Plimpton, 2005) (Schlick, 2002), etc. The MD simulation code (LAMMPS (Plimpton, 2005)) used in this study employs the velocity verlet scheme (described by Eqs. 5-8 below) to simulate the tensile and flexural deformation behavior of nanowires.

$$X(t+\delta t) = X(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2 + \mathrm{O}(\delta t^3) \quad (5)$$

$$v(t+\frac{\delta t}{2}) = v(t) + \frac{1}{2}a(t)\delta t + \mathrm{O}(\delta t^2) \quad (6)$$

$$a(t+\delta t) = -\frac{\nabla \Pi(X(t+\delta t))}{m} \quad (7)$$

$$v(t+\delta t) = v(t+\frac{\delta t}{2}) + \frac{\delta t}{2}a(t+\delta t) \quad (8)$$

(5) During the simulation of dynamic systems, the velocities of atoms need to be updated constantly to make the temperature of ensemble stable. The commonly used consistency strategies are velocity scaling, Langvin "white" noise, Berendsen friction, and Hoover/Nose's (Frankel & Smit, 2001) (Haile, 1997) (Schlick, 2002). Velocity scaling is used to maintain the temperature in this work on the tensile and flexural deformation of Nickel nanowires.

Molecular dynamics is a great tool, but there are limitations. Due to its high computational cost for large time-scale and length-scale problems, molecular dynamics method is only applicable for small scale problems. With the availability of parallel computing systems, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) (Plimpton, 2005), an efficient parallel MD simulation code developed by Sandia National Lab is employed. A brief description of LAMMPS is presented next.

2.1 Major Features of LAMMPS

The MD simulations require keeping track of the nearby particles of each atom. For computational efficiency, LAMMPS uses Verlet neighbor lists (Chialvo & Debenedetti, 1990) (Frenkel & Smit, 2001) (Rapaport, 1997) to keep track of nearby particles. As an extension of cutoff-radius methods, Verlet neighbor methods set neighbor cutoff radius as potential cutoff plus a "skin". The updating will not be triggered till a molecule travels a distance greater than the skin thickness. In this way, the updating of neighbor list (Chialvo & Debenedetti, 1990) becomes much less frequent. In this work, the skin size is set to be 0.03 (Plimpton, 2005).

On parallel, multi-processor computing systems, LAMMPS uses spatial-decomposition techniques (Plimpton, 2005) to partition the simulation domain into smaller 3D sub-domains. Each sub-domain is assigned to each processor. Processors communicate and store "ghost" atom information (Plimpton, 2005) for atoms that border their sub-domain.

A single macroscopic state that consists of different microscopic states is defined by an ensemble (Plimpton, 2005). Ensembles with specific characteristics that can be defined in LAMMPS include:

- Microcanonical ensemble (NVE): The thermodynamic state is characterized by a fixed number of atoms, *N*, a fixed volume, *V*, and a fixed energy; *E*. NVE corresponds to an isolated system.

- Canonical Ensemble (NVT): This is a collection of all systems whose thermodynamic state is characterized by a fixed number of atoms, *N*, a fixed volume, *V*, and a fixed temperature, *T*.
- Isobaric-Isothermal Ensemble (NPT): This ensemble is characterized by a fixed number of atoms, *N*, a fixed pressure, P, and a fixed temperature, *T*.
- Grand canonical Ensemble (mVT): The thermodynamic state for this ensemble is characterized by a fixed chemical potential, m, a fixed volume, *V*, and a fixed temperature, *T*.

In this work, NVE ensemble is employed for the tensile and flexural deformation behavior of Nickel nanowires.

In the molecular dynamics simulations, periodic boundary conditions are commonly used to enable representing infinite size material configurations with only a small number of atoms. The particles do not interact across the boundary and do not move out of their enclosed periodic box. Such periodic boundary conditions are generally used with LAMMPS. However, to simulate the tensile and flexural behavior of Nickel Nanowires in this work, the molecular system is set to be non-periodic.

2.2 Stress Definition in MD (Virial Stress)

Cauchy stress, which represents force per unit area of the deformed solid, is commonly used in classical mechanics problems (Frankel & Smit, 2001) (Haile, 1997). However, this is not applicable for discrete systems such as those in molecular dynamics problems. LAMMPS uses virial stress (Zhou, 2003) (Zimmerman et. al., 2003) to describe the macroscopic (continuum) stress in accordance with the microscopic quantities. Given the phase status of atoms, the macroscopic stress tensor in a macroscopically small, but microscopically large volume Ω is given by (Zhou, 2003) (Zimmerman et. al., 2003):

$$\sigma_{\alpha\beta} = \frac{1}{\Omega}\sum_{i\in\Omega}\{-m_i(v_{i,\alpha}-\bar{v}_\alpha)(v_{i,\beta}-\bar{v}_\beta)+\frac{1}{2}\sum_j(X_{j,\alpha}-X_{i,\alpha})f_{ij,\beta}\} \quad (9)$$

where

$$f_{ij,\beta} = \frac{\partial \Pi_i}{\partial X_j} \quad (10)$$

Here m_i is the mass of the i-th molecule in Ω, X_i is its position (α and β indicates Cartesian components), v_i its velocity, ū the local average velocity, and f_{ij} is the force on molecule i exerted by another molecule j. This virial stress is used to compute the stress values for the tensile and flexural deformation behavior in the present simulations.

3. Tensile Deformation of Nickel Nanowires

The strain-stress relationship and the tensile deformation behavior of Nickel nanowires investigated via MD simulations are presented next. The effect of temperature, strain rate and specimen size on the mechanical properties (e.g., the maximum yielding stress and Young's modulus) are studied and discussed.

3.1 Computational Model Configuration of Tensile Nickel Nanowires

Figure 2 shows the computational model configuration of Nickel nanowires used in this work. The Nickel nanowires are made of Nickel FCC crystals with initial surface orientation of <100>, <010> and <001> (Liang & Zhou, 2003). The lattice constant of faced-centered cubic (FCC) (Frankel & Smit, 2001) (Haile, 1997) (Schlick, 2002) Nickel crystal is ג=3.52 Å.

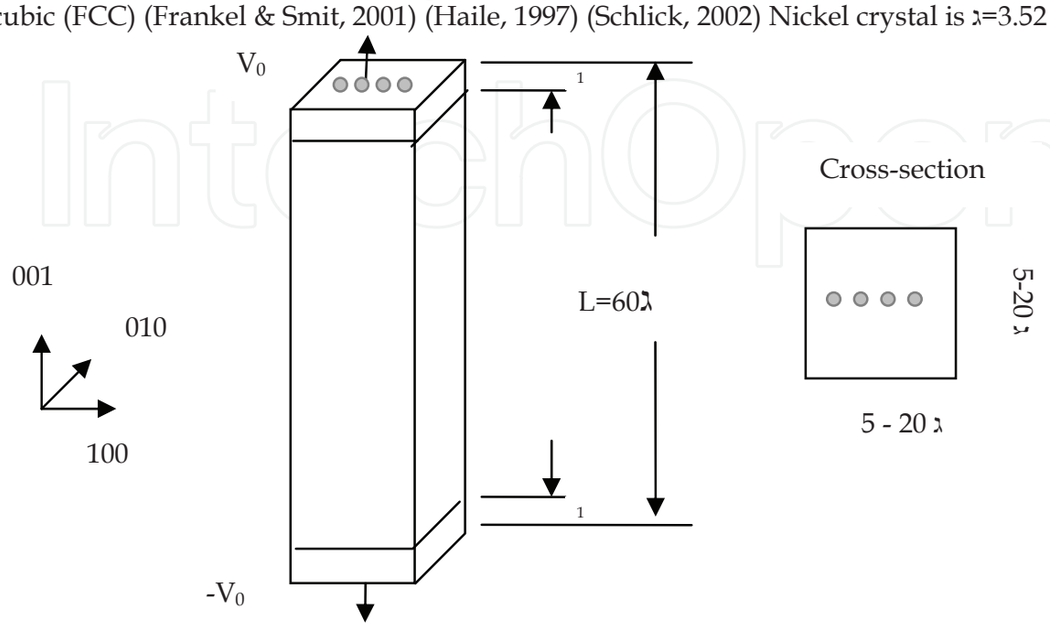


Fig. 2. Configuration of Tensile Nickel Nanowires for Tensile Deformation

In this work, the length (L) of Ni nanowires was set to be 60ג in the <001> directions for the MD simulations of the tensile deformation behavior. Different cross-sectional sizes that range from 5 to 20 ג for a side formed the different Nickel nanowire configurations. Constant velocities $\pm V_0$ are enforced on the top and bottom layers of the nanowires. These top and bottom layers define the boundary layer and have identical size of 1 lattice constant, along the <001> crystalline direction.

Based on the velocities over boundary layers ($\pm V_0$), the nanowire model system deform under strain rate given by:

$$\varepsilon' = \frac{2V_0}{L} \quad (11)$$

Here L is the length of Nickel Nanowires (Liang & Zhou, 2003).

Different velocities were employed in the simulations to give different strain rate conditions. Table 1 shows the velocity of boundary layers (V_0) and the resulting strain-rate. It should be noted that in LAMPPS the velocity is always expressed as lattice-constant (ג) per pico-second.

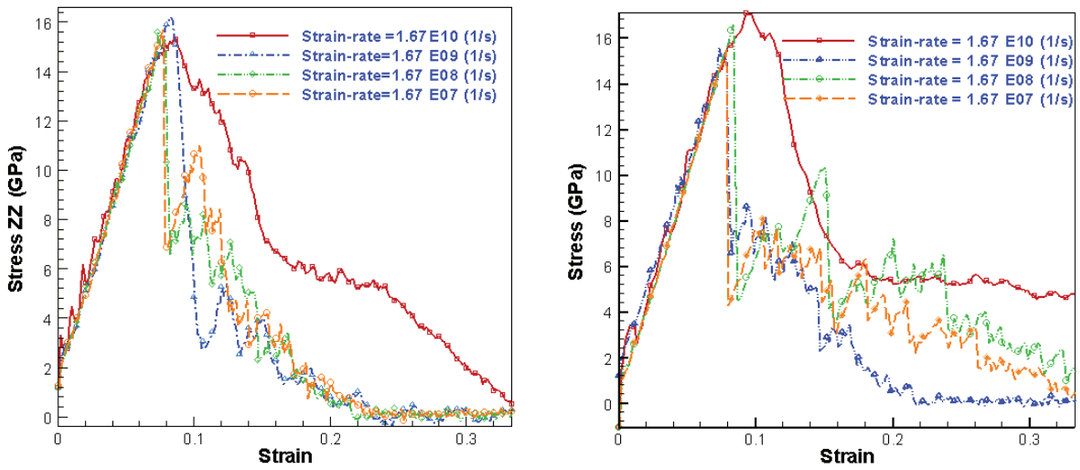
$\dot{\varepsilon}$(1/s)	V_0 (Å/ps)
1.67×10^{7}	5×10^{-4}
1.67×10^{8}	5×10^{-3}
1.67×10^{9}	5×10^{-2}
1.67×10^{10}	5×10^{-1}

Table 1. Tension Velocity of Nickel Nanowires and the Resulting Strain Rate

The tensile behavior of Ni nanowires and the influencing factors investigated through the MD simulations are presented next.

3.2 Effect of Strain Rate

Figure 3 presents the tensile stress-strain behavior obtained from 5×5×60 and 10×10×60 Nickel nanowires at various strain rates (1.67×10^{7} – 1.67×10^{10} s^{-1}). These simulations are based on an NVE ensemble at temperature T=*300K*. It is observed that a higher strain-rate led to higher oscillations in the stress-strain curve.



(A) 5×5×60; (B) 10×10×60

Fig. 3. Stress-Strain Curve of Nickel Nanowires under Various Strain-rates at T=300K.

The Young's modulus is determined from the results of tensile stress – strain curve for the strain $\varepsilon < 0.08$ using a linear regression. Table 2 and 3 shows the Young's modulus and maximum yielding stress of Nickel nanowires respectively under tensile loading.

Strain-rate($\dot{\varepsilon}$)	5×5×60	10×10×60
1.67×10^{7}	191.27	184.2127
1.67×10^{8}	189.82	192.0556
1.67×10^{9}	184.33	190.3636
1.67×10^{10}	182.71	187.2973

Table 2. Young's Modulus (GPa) of Nickel Nanowires for Various Strain-rates

This data indicates that strain rate does not significantly influence the Young's modulus and the maximum yield stress.

Max. Yielding Stress (GPa)	5×5×60	10×10×60
1.67×10^{7}	15.7178	15.4835
1.67×10^{8}	15.6100	16.6046
1.67×10^{9}	16.2640	15.6100
1.67×10^{10}	15.3314	17.0836

Table 3. Maximum Yielding Stress (GPa) of Nickel Nanowires for Various Strain-rates

Figures 4 and 5 present the progressive deformation and failure of 5×5×60 Ni nanowires for the strain rates $1.67x10^{7}$ and $1.67x10^{10}$ (s^{-1}) respectively. As seen from these results, it is observed that the yielding slip planes, cross slip and the breaking neck (Chang & Fang, 2003) (Schlick, 2002) (Silva, et. al., 2004) of Nickel Nanowires are influenced by the strain-rate. The two deformation configurations presented in figures 4 and 5 are an intermediate configuration during the deformation and the final yielding configuration. These figures clearly show that the strain rate influences the yielding slip planes, cross slip, and the breaking neck of the Ni nanowires.

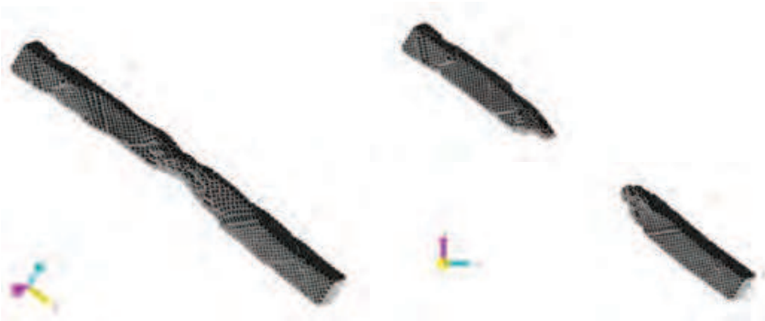


Fig. 4. Tensile Deformation and Failure of 5X5X60 Nickel Nanowire; Strain Rate = 1.67×10^{7} (s^{-1})

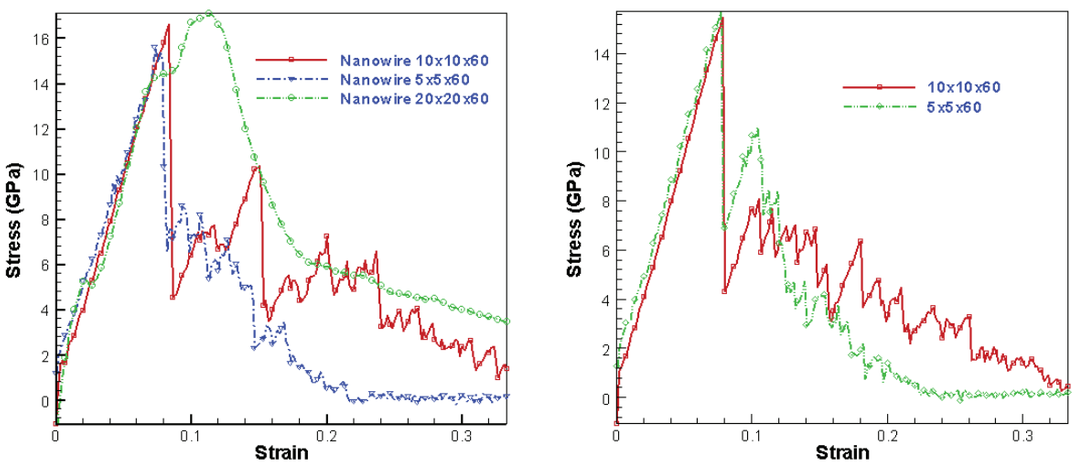
Fig. 5. Tensile deformation and failure of 5×5×60 Nickel nanowires; strain rate=1.67×10^{10} (s^{-1})

3.3 Effect of Nanowire Cross Section Size

For a specific strain-rate (1.67×10^{10} s^{-1} or 1.67×10^{7} s^{-1}), Figure 6 presents the comparison of the simulated strain-stress behavior of Nickel nanowires for varying cross-sectional dimensions (5-20 ג) (Liang & Zhou, 2003). The results indicate that cross-sectional dimension does not significantly affect the Young's modulus of Nickel Nanowires. The larger cross-sectional dimension leads to larger maximum yielding stress. Further, it is observed from Figure 6 that larger cross-sectional dimension nanowires have less numerical oscillations

amplitude compared to the smaller cross-sectional dimension nanowires. This phenomenon may be caused due to the dynamic wave effect or phonon drag that impedes the motion of dislocations (Liang & Zhou, 2003).

Table 4 and 5 shows the Young's modulus and maximum yielding stress of tensile Nickel nanowires, respectively for various cross-sectional dimensions. These results indicate that the cross-sectional size does not significantly affect the Young's modulus and the maximum stress obtained from the simulations.



(A) strain-rate = 1.67×10^{10} s^{-1} (B) strain-rate = 1.67×10^{7} s^{-1}

Fig. 6. Strain-stress curve of Nickel nanowires for Various cross-sectional dimensions

Strain-rate($\dot{\varepsilon}$)	5×5×60	10×10×60	20×20×60
1.67×10^{7}	191.27	184.2127	-
1.67×10^{10}	182.71	187.2973	184.0893

Table 4. Young's Modulus (GPa) of Nickel Nanowires for Various Cross-sectional Dimensions

Strain-rate($\dot{\varepsilon}$)	5×5×60	10×10×60	20×20×60
1.67×10^{7}	15.7178	15.4835	-
1.67×10^{10}	15.3314	17.0836	17.1271

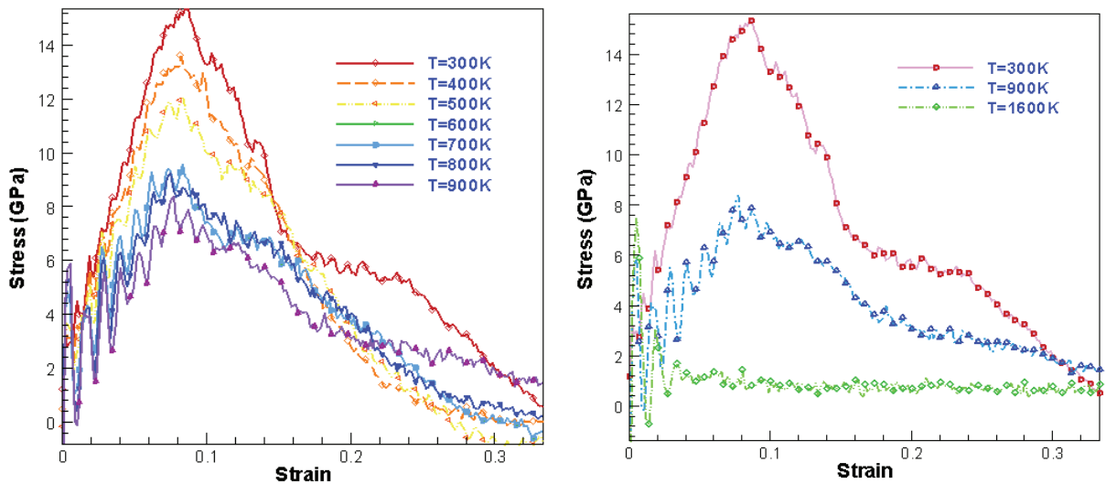
Table 5. Maximum Yielding Stress (GPa) of Nickel Nanowires for Various Cross-sectional Dimensions

3.4 Effect of Temperature

Temperature plays an important role in the deformation behavior of nanomaterial systems. Molecular dynamics simulations as presented and discussed in this chapter provide an effective predictive methodology to understand the deformation behavior of nanomaterial systems (such as the nanowire). This section focuses on the effect of varying temperature on the mechanical properties and deformation behavior of Nickel nanowires (Chang & Fang, 2003). For this analysis, molecular dynamics simulations are performed for various temperature conditions of the molecular ensemble. Figure 7(A) shows the stress-strain behavior at temperature ranging from 300K to 900K in steps of 100K. Figure 7(B) includes

the stress-strain behavior at a higher temperature of 1600K which is close to the melting point of Nickel (1728K) along with the behavior at room temperature (300K) and an elevated temperature (600K). The simulated stress – strain deformation behavior obtained from Figure 7(A) indicates that:

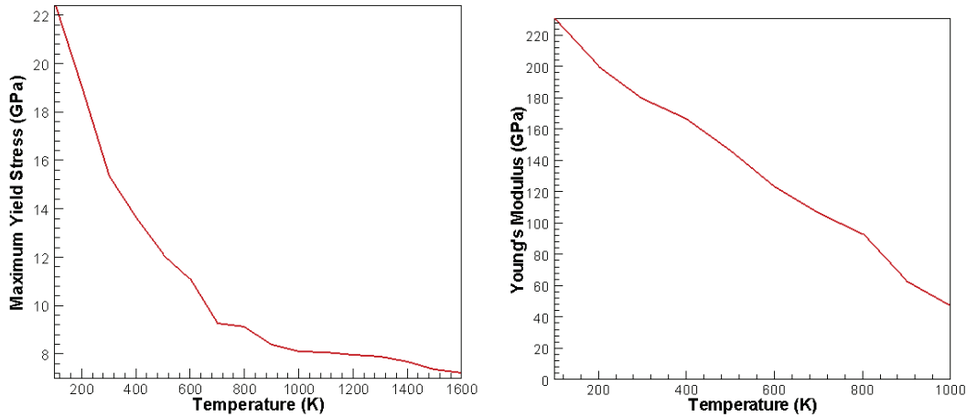
- The maximum yielding stress decreases as the temperature of the ensemble increases
- With the increase of ensemble temperature, the thermal oscillations due to numerical corrections and temperature scaling also become dominant.



(A) In the temperature range 300-900K (B) Near melting point.

Fig. 7. Stress-Strain behavior of 5×5×60 Nickel nanowires at various temperatures

Figure 8(A) shows the change in the maximum yield stress of Nickel nanowire at varying temperatures ranging 100K-1600K. As can be expected, the maximum yield stress decreases with increasing temperature. Figure 8(B) shows the associated Young's modulus of Nickel nanowires obtained from molecular dynamics simulations at various temperatures. As seen from this figure, the Young's modulus of Nickel nanowires decreases fairly linearly as the temperature increases.



(A) Maximum yield stress (B) Young's modulus

Fig. 8. Effect of Temperature on the Maximum Yield Stress and Young's Modulus of Nickel Nanowires (5×5×60)

Figure 9 illustrates the superior ductility of Nickel nanowires around melting temperature. As seen from figure 9 obtained from the molecular dynamics simulations, it is observed that when the ensemble is maintained at 1600K, the nanowires can be greatly extended without a ductile fracture. Further discussions of molecular dynamics simulations on the transition from brittle to ductile are presented in Cheung and Yip (Cheung & Yip, 1994).

Fig. 9. Deformation configuration of 5×5×60 Nickel nanowire at T=1600K

4. Flexural Deformation of Nickel Nanowires

This section focuses on the flexural deformation behaviour of Nickel nanowires due to flexural bending based on their molecular configurations using molecular dynamics simulations. In particular, the deformation vibration frequencies obtained from the molecular dynamics simulations are compared with the natural frequencies based on classical beam theory for two different boundary conditions.

4.1 Computational Model Configuration and Analysis of Flexural Nickel Nanowires

Figure 10 presents the configuration of Nickel nanowire beams and the corresponding molecular model. The molecular model configuration is based on single crystals of Nickel in the <001> (longitudinal direction), <010> and <100> (transverse directions) directions and with a dimension of 120×10×1 cubic lattice constants (rectangular cross section with a longer span). Two types of boundary conditions are employed in the simulations: 1. Both ends pinned (i.e., simply supported), 2. Both ends clamped. The nanowire beam deflects under the action of applied loading and when the loading force is removed, the displaced beam would try to return to its original position. The inertia of the beam would cause the beam to vibrate. The transient flexural bending dynamic behavior of the molecular configuration of Nickel nanowire beams are investigated and analyzed.

The transient molecular dynamic simulations compute the new position of the atoms in the Nickel nanowire beam subjected to the flexural loading and the boundary constraints. The time increments are however significantly small in these dynamic simulations. A Mean Square Displacement (MSD (u(t))) is defined and used as a measure of the average distance an atom in the model travels over a certain time interval period. This is defined as:

$$msd(u(t)) = \frac{1}{N}\sum_{i=1}^{N} u_i^2(t) = \frac{1}{N}\sum_{i=1}^{N} (r_i(t) - r_i(0))^2 \tag{12}$$

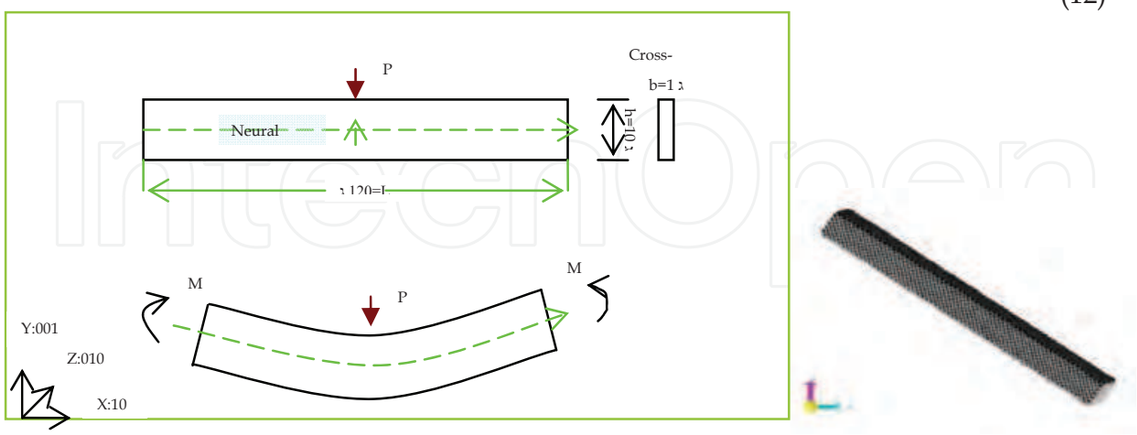


Fig. 10. Configuration of Nickel Nanowire Beams for Flexural Deformation and Molecular Model

The displacement $\boldsymbol{u}_i(t)=\boldsymbol{r}_i(t)-\boldsymbol{r}_i(0)$ is the distance traveled by molecule i over some time interval t, and the squared magnitude of this vector is averaged over many such time intervals. This MSD displacement value is used in the analysis of time dependent displacement response of the Ni nanowires. The dynamic displacement response under two different boundary conditions for flexural bending is studied.

4.2 Simply Supported Nickel Nanowire Beam

The Nickel nanowire beam configuration as shown in figure 10 is simply supported (rotations are possible at the ends) and is subjected to a dynamic concentrated point load at the center of the nanowire beam. Two different load values (F=0.01eV/Å and 0.03eV/Å) are analyzed.

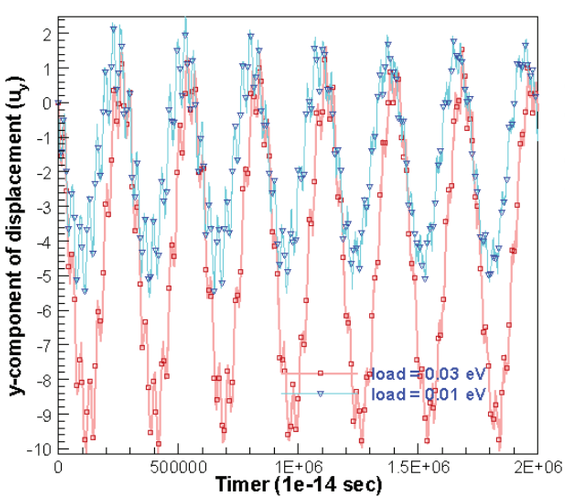


Fig. 11. Transient Dynamic Vertical Displacement at the Center (simply supported ends)

Figure 11 presents the dynamic mean square vertical displacement variation with time at the center of the nanowire beam under these two loading conditions. These are based on the averaged vertical displacement of the atoms in the cross-sectional plane at the center in all cases.

The dynamic vertical displacement at the center is proportional to the loading value and increases with a higher magnitude of external loading. The natural frequency of the dynamic vibration as computed from the displacement - time profile is however independent of the magnitude of external loading. The computed angular frequency from the predicted time dependent deflection of the molecular model of the Nickel nanowire beam shown in Figure 11 is 2.4166E+09 Hz.

The natural frequency for the case of a simply supported beam based on classical beam theory analysis is given by (Megson, 1996) (Voltera & Zackmanoglou, 1965) (Tedesco et. .al., 1999)

$$\omega_n = (n\pi)^2 \sqrt{\frac{EI}{\rho A L^4}} \tag{13}$$

Using a Young's Modulus value of E = 190 GPa (1.1859 eV/A^3) obtained from molecular dynamics modeling of the tensile stress strain deformation of Nickel nanowires discussed in the earlier section, the mode 1 frequency value obtained from the classical beam theory is 2.5244E+10 Hz. This frequency as obtained from the classical beam theory is at least one order higher than the frequency obtained from the time dependent deflection using molecular dynamics simulations. The classical elastic beam theory based on continuum mechanics principles also indicate that the natural frequency of vibration of a simple supported beam is independent of the magnitude of the external loading and depends only on the beam cross sectional moment of inertia, cross-sectional area, length and modulus of elasticity of the material. The natural frequency obtained from molecular dynamics simulations for the loading and simply supported boundary conditions as presented in figure 11 is also independent of the magnitude of the external loading.

4.3 Clamped Nickel Nanowire Beam

The previous section considered the case of a simply supported boundary condition configuration where the rotation at the ends of the flexural beam is permitted. The same nanowire beam is fixed at both ends (displacement and the rotation at the ends are zero) and is subjected to external loading force at the center. As before, two different loading values are investigated. Figure 12 presents the computed dynamic displacement response of the loaded center of the nanowire beam. As seen from figure 12, the dynamic displacement magnitude depends on the external loading value while the frequency of the dynamic displacement is independent of the external loading values. This is in direct correlation with the analytical results of natural frequency based on the classical beam theory.

The computed angular frequency obtained from the predicted time dependent deflection of the clamped Nickel molecular beam shown in Figure 12 is 2.3271E+09 Hz. The frequency of vibration based on the classical beam theory for this case of clamped ends is given by (Megson, 1996) (Voltera & Zackmanoglou, 1965) (Tedesco et. .al., 1999)

$$\omega_n = (K_1 L)^2 \sqrt{\frac{EI}{\rho A L^4}}; \quad K_1 = 4.73 \tag{14}$$

Using the same Young's Modulus for the Nickel nanowire as before, the mode 1 natural frequency as obtained based on the classical beam theory is 5.7225E+10 Hz. This frequency obtained from the classical beam theory for this clamped Nickel nanowire beam configuration is at least one order higher than the frequency obtained from the time dependent center point load deflection using the molecular dynamics simulations. The classical beam theory based on continuum mechanics principles also indicate that the natural frequency of a clamped beam is independent of the external loading and depends only on the beam cross sectional moment of inertia, cross-sectional area, length, and modulus of elasticity of the material. This was also the case in the frequency of the nanowire beams obtained from molecular dynamics simulations as presented in figure 12.

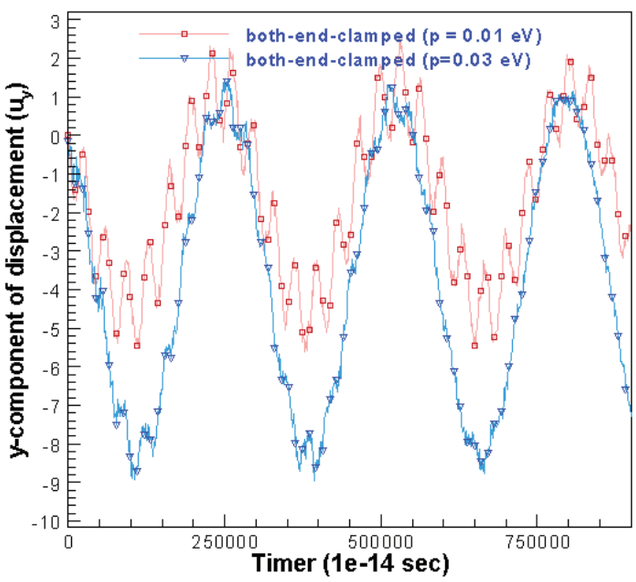
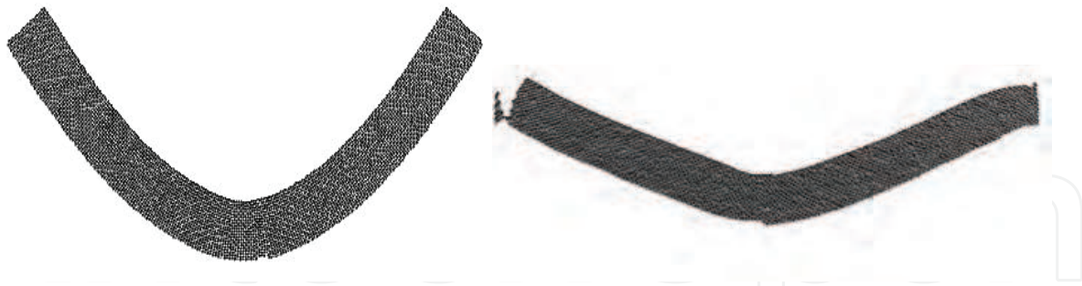


Fig. 12. Transient Dynamic Vertical Displacement at the Center (clamped ends)

4.4 Effect of Large Loading

The flexural, bending failure behavior of these Nickel nanowire beams with a larger loading is studied. As the loading is increased, the failure profile from the molecular dynamics simulations clearly shows the effect of boundary conditions. A shear slip failure along the mid-plane at the center of the nanowire beam where the shear forces are higher is seen in the case of nanowire beam with the clamped ends. The simply supported nanowire beam configuration presents a similar failure at the center of the nanowire beam but did not show predominant shear slip failure. Figure 13 shows the deformed shape at failure with a larger load for both the boundary condition cases discussed earlier. Molecular dynamics modeling provides effective means of understanding the deformation of Nickel nanowires using the molecular model configuration. These simulations are effective in understanding the deformation and failure behavior of these material systems and are especially useful as the

experimental techniques are not practical and conducive for such length scale material systems.



(A) Simply Supported Ends. (B) Clamped Ends

Fig. 13. Deformed Shape on Failure (left: simply supported; right: clamped)

5. Summary and Concluding Remarks

As the metallic nanowires are increasingly used in electronic devices, it is essential to understand their mechanical deformation behavior, structural and mechanical stability under external mechanical and thermal loading conditions. This mechanical strength and stability are important considerations during the life cycle of these electronic devices, as well as in other applications of such metallic nanowires. Computational modeling and simulations based on molecular dynamics modeling and the associated inter atomic potential provide an effective means to understand these mechanical behaviors. These computational modeling and simulations are based on the molecular model configurations of these metallic nanowires. In this chapter, molecular dynamics modeling of the two fundamental mechanical behaviors of Nickel Nanowires, namely the tensile deformation and failure of Nickel nanowires; and the flexural bending deformation behavior of Nickel nanowire beam configurations are presented and discussed. The tensile deformation behavior focused on the stress-strain behavior and the tensile failure of the nanowires. The flexural deformation behavior focused on the vibration characteristics of the nanowire beams subjected to external loading and its release. Nanowire inter-connectors in electronic devices often are subjected to such loading conditions and these enabling molecular computational modeling and simulations for nanotechnology applications provide an effective means for such analysis.

The molecular dynamics simulations for the tensile mechanical deformation behavior in Nickel nanowires employed the molecular configurations of Nickel (FCC crystal structure). The deformation behavior of these atomic molecular configurations is modeled based on the force field interactions between the Nickel atoms at a finite temperature. These simulations are conducted using a classical molecular dynamics code LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator) from Sandia National Laboratory. The force field interactions between the Nickel atoms are modeled based on the embedded atom potential (EAM).

Molecular dynamics modeling of the tensile behavior of Nickel nanowires under different strain rates were conducted to predict the stress-strain behavior and Young's Modulus of these nanowires. The tensile deformation behavior indicated that the Young's Modulus was independent of the cross sectional area of the nanowire and the strain rate employed in the tensile deformation. Also, as the temperature increases, the Young's modulus of Nickel

nanowire is found to decrease with improved ductility. At a temperature close to the melting temperature, the molecular Nickel nanowire configuration behaves as a highly ductile, fluid material system.

The bending and flexural deformation and vibration behavior indicated that the frequency of the vibrations as compared from time displacement deformation behavior of the molecular configurations of the Nickel nanowire beams are independent of the magnitude of external loading. This was the case for both the simply supported and clamped end boundary configurations discussed in this chapter. This is consistent with the natural frequency based on the classical beam theory for such boundary and loading conditions. The magnitude of natural frequency was however higher when compared with the classical beam theory. The displacement magnitude was also significantly higher in the case of a larger loading. A higher loading however causes the failure of the simulated Nickel nanowire beam. A shear-slip type of failure along the mid plane at the mid-point of the beam was observed with a larger bending flexural loading. This shear-slip failure is predominant in the case of the clamped boundary condition.

Experimental investigations of the mechanical behavior of metallic nanowires are impractical and computational molecular modeling and simulations as analyzed and discussed in this chapter provide effective means for such analysis.

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The main purpose of this book is to describe important issues in various types of devices ranging from conventional transistors (opening chapters of the book) to molecular electronic devices whose fabrication and operation is discussed in the last few chapters of the book. As such, this book can serve as a guide for identifications of important areas of research in micro, nano and molecular electronics. We deeply acknowledge valuable contributions that each of the authors made in writing these excellent chapters.

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