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Atomistic Simulation of the Effect of Temperature on Mechanical Properties of some Nano-Crystalline Metals

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Abstract

For materials with high ductility, malleability and conductivity, temperature will have significant impact on the material properties. This is especially true for pure elemental metals which have a wide range of applications due to their ultrahigh strengths. Recently, the study of damage mechanism at the nano- and micro level has attracted a significant interest and research. However, the current understanding of deformation mechanisms in nanocrystalline metals in relation to atomic structure and behavior is insufficient. In this study, atomistic simulation of uniaxial tension at nano-scale was performed at a fixed rate of loading (500 ms^{-1}) on some nano-crystalline face centered cubic metals (Al, Cu, and Ni), to study the nature of tensile deformation at different temperatures using the embedded-atomic method (EAM) potential function. The simulation results show a rapid increase in the stress up to a maximum value followed by a sharp drop when the nanocrystal fails by ductile dislocation. The drop in the stress-strain curves can be attributed to the rearrangement of atoms to a new or modified crystalline structure. Additional simulations were run to study the effects of temperature on the stress-strain curve of nano-crystals. The result shows that increasing temperature weakens the ductility of these nanomaterials. In this investigation, the strain corresponding to yielding stress is observed to be lower with increasing temperature. Finally, the evolution of crystalline microstructure during the entire tensile process was investigated. The atomistic simulation result of tensile deformation at nanoscale obtained in this study agree with plasticity phenomenon observed in macroscale.

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Keywords: Molecular dynamics, Tensile deformation, Ductility, Nanocrystalline metals, Plasticity

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1. Introduction

At present, there is a growing interest in understanding the mechanical properties of micro-and nanosized structures due to their wide applications in the development of micro-electromechanical systems (MEMS) and nanoelectromechanical systems (NEMS) [1-6]. These micro and nano components are capable of withstanding complex stress with little risk of failure. Such materials are created through processes that result in no or very few defects. As a result, it is necessary to investigate the structural mechanics behavior of defect-free nanomaterials. Generally, to experimentally determine the mechanical properties of nanomaterials is difficult, if not impossible. An alternative approach is atomic simulation techniques. Atomistic simulation is typically performed on a finite number of atoms within a variable-size computational cell, with precise boundary conditions and other constraints such as temperature, stress, and strain. In this regard, techniques that access the molecular level, such as Molecular dynamics (MD) and Monte Carlo (MC), are highly effective for atomistic modeling of materials.

Molecular dynamics (MD) is a computer simulation technique that tracks the evolution of a system at the atomic level, making it ideal for describing materials at the atomic scale [7]. The classical MD simulations method, in particular, has previously been used to study a range of realistic systems with various force fields. Among these are investigations into pure metals such as sodium [8-9], potassium [10], rubidium [11], and binary metals-alloys [8, 12]. Recently, MD simulation technique has become a useful tool to study the mechanical properties and deformation behavior of materials at the nano or atomistic regime [13-15]. Heino *et al.* [16], simulated strain on a single Cu crystal for various orientations using MD simulations. They found that the calculated and experimental tensile moduli differed by 2-6% and 3-15% respectively. Zhou *et al.* [17], investigated the deformation mechanisms of nanocrystalline copper using molecular dynamics simulations. Chang *et al.* [18-19] employed molecular dynamics simulations to study the tensile behavior of single crystal titanium for different strain rates ($108\ s^{-1} - 1011\ s^{-1}$). Komanduri *et al.* [20], used Morse potential to simulate uniaxial tension of some single crystal cubic metals. In the simulation, necking was observed. More specifically, MD simulation was used at the nanoscale level to simulate the elasto-plastic behavior of monocrystals in various orientations. Rosandi *et al.* [21], investigated the mechanical properties of Al nanowires and alumina coated Al under tension and compression at various strain rates. Liang & Upmanyu [22], studied the size dependent elasticity of copper nanowires using a molecular statics methodology based on the embedded atom method (EAM) potential. Yuan *et al.* [23], used the Morse potential to investigate the tensile process of nano-single crystal Al at various strain rates and temperatures. Their results show that the stress–strain curves increase linearly up to the maximum value, then slowly drops. The phenomena can be attributed to the first transition from elastic to plastic deformation. Li *et al.* [24], investigated the deformation behavior of nanocrystalline TiAl alloys under tensile loading conditions using MD simulations.

Although the above simulations were close to real system, the load paths used were far from the real load. Besides, most of the simulations were carried out at $0\ K$ or room temperature, and a few were conducted at various temperatures. Thus, it's important to understand how single nano-crystals deform at different temperatures. In this paper, atomistic molecular dynamics simulation was employed to study the tensile deformation behavior of three nano-single crystalline metals (Al, Cu and Ni), at different temperatures using a semi-empirical embedded atom model (EAM).

2. Methodology

2.1. Theory and Simulation Details

In this study, the embedded atom method (EAM) potential was employed in setting-up Molecular dynamics (MD) simulation. This many-body potential was specially developed for metals and has proven to be able to well describe the metallic bonding in crystals. The general form of the total potential energy of a system of atoms described by the EAM formalism is given by [25, 26].

$$E_{tot} = \sum_i F_i(\phi_i) + \frac{1}{2}\sum_i \sum_{j \neq i} \varphi_{ij}(r_{ij}), \tag{1}$$

where, F_i is a function of the effective electron density at atom i, ϕ_i .This many-body term can be interpreted as the energy it takes to embed atom i into effective electron density. The term $\varphi_{ij}(r_{ij})$ is a basic pair potential that is commonly used to describe electrostatic interactions. In his classic paper, Daw [27], established that EAM can be derived

starting from Density functional theory (DFT) arguments. Although, EAM potential typically require experimental data or *ab initio* calculations in order to determine specific parameters for the embedding energy, effective electron density, and pair potential. Therefore, this class of potential is often referred to as semi-empirical potentials.

Once the potential function is determined, the molecular force F_{ij} is calculated as the derivative of the potential energy, i.e.

$$F_{ij} = -\frac{\partial U(r_{ij})}{\partial r_{ij}}. \tag{2}$$

The velocity Verlet method was used as the integration algorithm. See ref. [28], for details of the velocity Verlet method. The velocity scaling method as described in ref. [29], was used to control the temperature. MD simulations were carried out using Large scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [30]. Ovito program was applied for visualization in the post-analysis of the simulation results [31].

2.2. Model of stress-strain

The MD simulations were performed in the canonical ensemble with the total number of particles N, volume, V, and temperature, T fixed using the velocity Verlet algorithm with time step of 0.01 fs. The tensile deformation simulations were based on single crystal aluminum (Al), copper (Cu), and nickel (Ni) lattice in the form of the fcc structure. The simulations started from a cubic shaped box with 10000 atoms. The Verlet numerical integration algorithm was used to determine the atomic position and velocity. The model consists of two parts. One part is designed to be the boundary zone where the positions of the atoms are subjected to periodic boundary conditions. A shrink-wrapped boundary was set in the two other directions. This means that the simulation box will deform in response to the motion of atoms. The position and velocity of the middle atoms will be updated using constant number of atoms, constant volume and constant energy (NVE), integration which keeps the volume and the energy of the system constant. The time steps of the simulation were set to 1 fs. The x, y, z coordinate axes represent the lattice direction of [100], [010] and [001] respectively. In order to simulate uni-axial tensile loading in the y-direction, the lower end of the nanocrystal is fixed, and a constant velocity increment is applied to all atoms in the upper end block. The interior atoms in the model were also given an initial y-velocity that varied linearly from 0.0 to the prescribed velocity at the top atomic plane depending on their y-coordinates in the simulation box to avoid the shock that would be induced into the block of material due to the high strain rates. The stress-strain curve was computed by calculating the stress per atom, then the stress per atom is summed for all the atoms in the simulation box in a selected direction and divided by the total system volume. To initialize the simulation, a relaxation state is defined and the atoms are left freely with a random velocity using NVT. Following initialization, simulations were carried out in a series of increasing temperatures from 100 to 900 K in 100 K increments.

3. Results and Discussion

3.1. Microstructure evolution of tensile deformation

To explore the inherent mechanisms of these deformations, the microstructure evolution with a strain rate of 500 ms^{-1} at 100 K was typically selected to study the microstructure transformation of Ni. A similar situation is found for the case of the other two metals investigated namely, Cu and Al. After relaxation, the symmetry of the surface atoms was broken which resulted to the rearrangement of atoms positions. Figure 1(b) shows a slight compressive bulge of the specimen after relaxation due to internal forces. The initial deformation of the nano-crystal is elastic. When the specimen stretches to a strain of 0.15, the first dislocation moves out from surface to create plastic deformation. This dislocation continue to occur, move and propagate with the strain as shown in Figure 1(b-c). The deformation will entirely localize into a very small neck region. This localization would likely permit very little additional macroscopic stretch. Towards the later stages, the deformation concentrates in the neck region (Figure 1d). The diameter of the neck was observed to constantly decrease as the deformation of the nanocrystals increases. Figure 1 shows that the atomistic simulation of tensile mechanisms at the nanometer scale produce results that are consistent with the mechanisms of plasticity found in macroscale experiments [32].

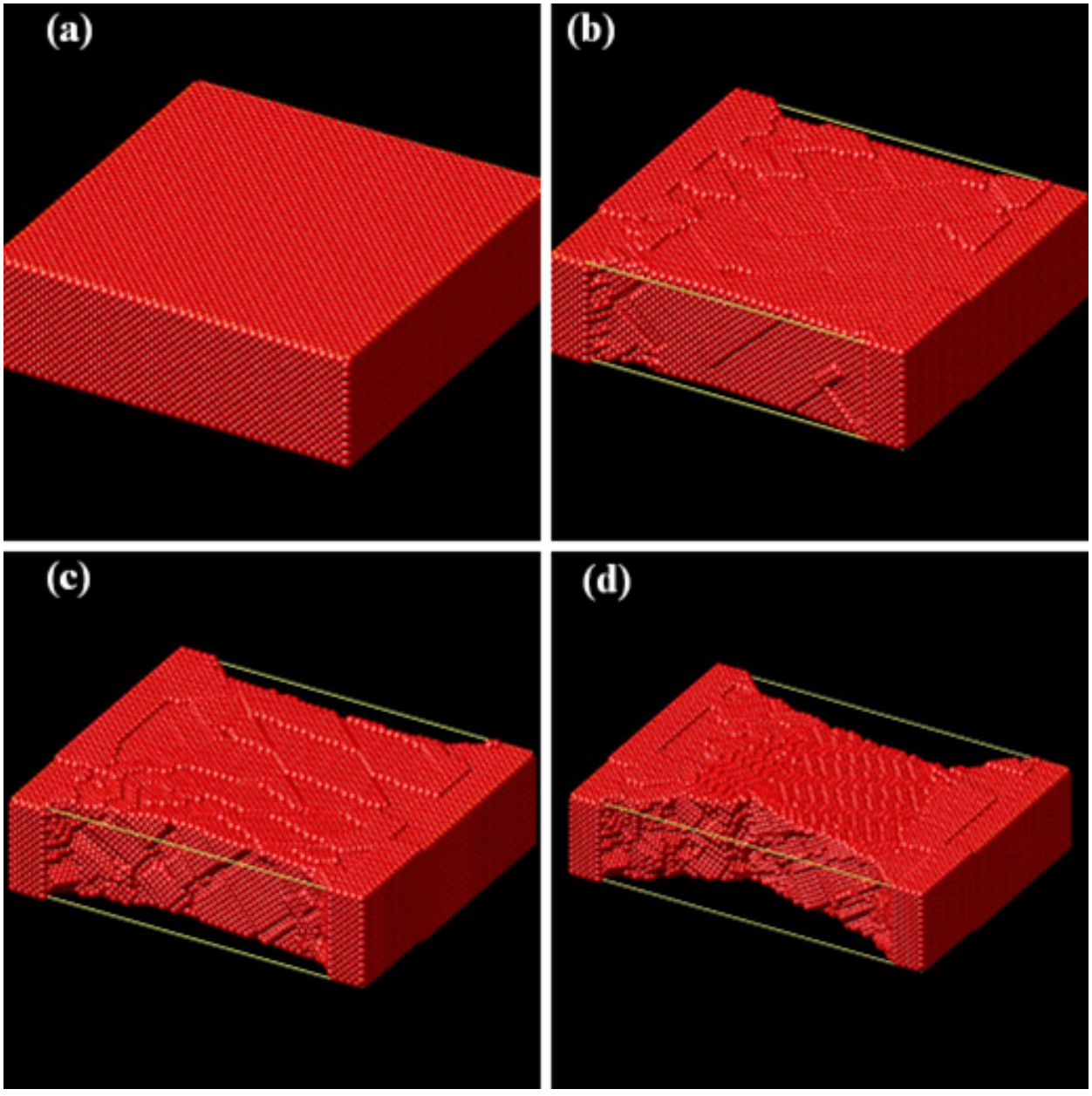

Figure 1. The snapshots of atomic configurations of nano-crystal aluminum 100 K and strain rate of 500 m/s.

3.2. Stress-strain curves at 100 *K and loading rate* 500 ms^{-1}

Figure 2 shows the stress–strain plots of the results obtained by MD simulation for single crystals of Al, Cu, and Ni. It can be seen that under tensile load, all three metals go through the similar deformation stages. The initial deformation is elastic in nature, followed by a rapid increase in the stress, up to the maximum stress of 3.5 GPa, 3.2 GPa, and 2.9 GPa, respectively for nickel, copper, and aluminum. Subsequently, the system enters the plastic deformation stage with a sharp drop in the stress. By comparing the maximum stress value of the stress–strain curve, it can be seen that the crystals' tensile strength decreases with increasing ductility, with Ni having the highest yield stress, followed by Cu and Al, as expected given their ductility. In contrast to conventional tensile testing, where the stress–strain diagram is essentially smooth with a linear slope in the elastic region, after entering the plastic region, the

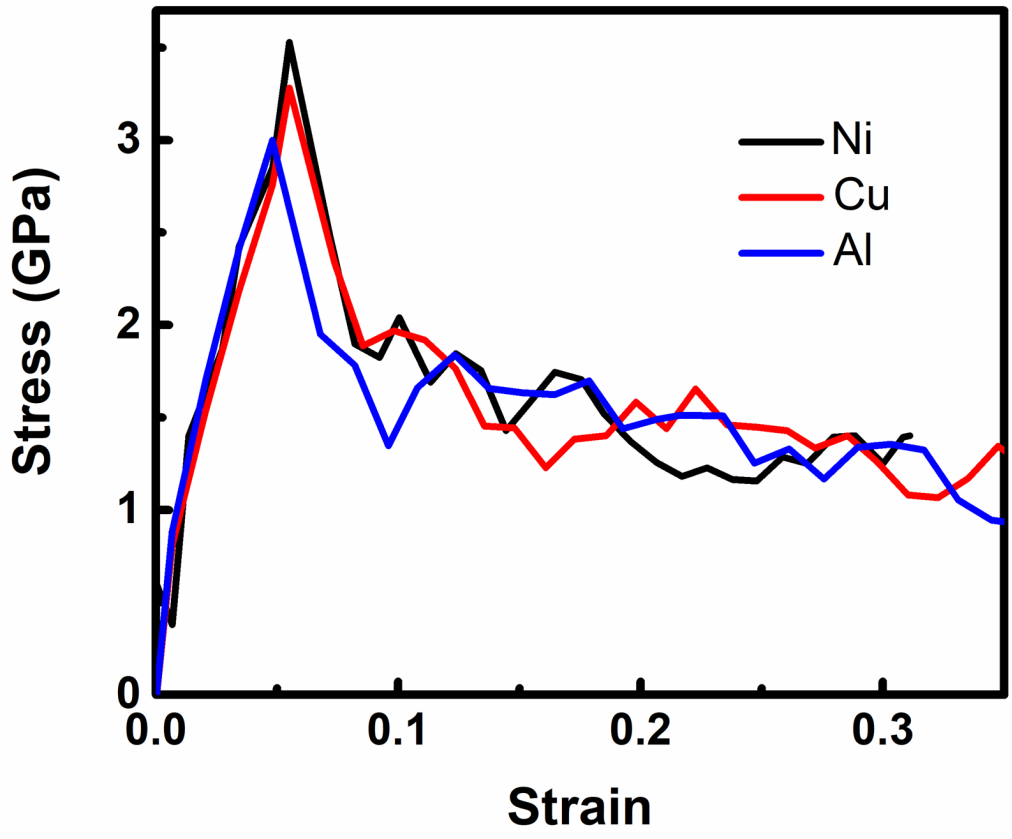

Figure 2. Stress–strain diagrams obtained by MD simulation of the tensile specimens of various materials, namely, Al, Cu, Ni.

tail of this stress–strain curve is characterized by a series of steps of rise and fall in the values, suggesting irreversibility of the process, which is in good agreement with the theory [21, 33]. The phenomenon can be explained by the initial transition from elastic to plastic deformation.

3.3. The effect of temperature on stress-strain and yield strength and yield strain

One of the most important factors that influences materials properties is temperature. In this section, the deformation behaviors of Al, Cu, and Ni nano-crystals were studied at temperatures of 100, 300, 500, 700, and 900 K with a constant strain of 500ms-1. It can be seen that at different temperatures, all the specimen undergo the same deformation process, which are the elastic deformation in the initial stage followed by plastic deformation stage. The peak (maximum stress value), of the stress-strain curve increases with reducing temperature (see Figure 3), indicating that increase in temperature leads to decrease in stress which is caused by the amount of dislocation occurring during the deformation process. In Figure 3, it is interesting to see that apparently more dislocations formed in nanocrystals under higher temperatures than those of lower temperatures. It is worth noting that the stress-strain curve for all the specimen show a similar trend under temperature variations. This behavior can be attributed to the weakening ductility of the nanomaterials. A microstructural analysis of appear to result in lower ductility. The three most common metrics for ductility are uniform elongation, total strain at failure, and area reduction. For all specimen, the uniform elongation, or the strain at peak load, was typically ~ 6% and the total strain at failure was approaching 10%.

In this study, the peak of the tensile stress-strain curve was used to represent the yield strength [34], which signifies

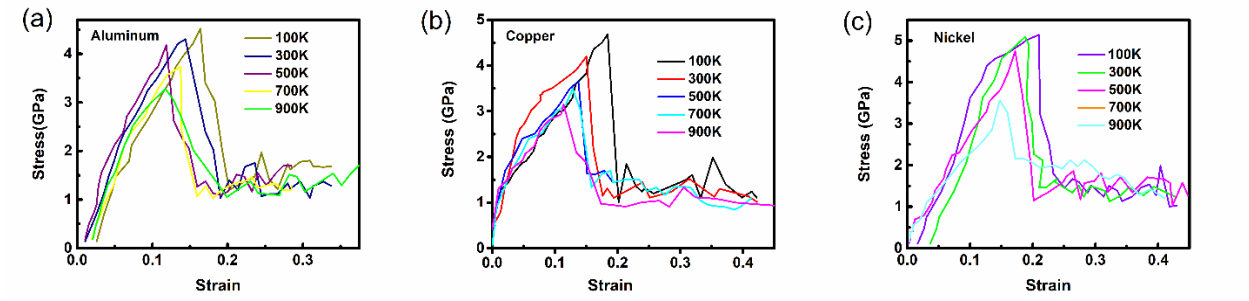

Figure 3. Stress-strain curves at different temperatures (100-900 K) and loading 500 m/s loading rate for (a) Al (b) Cu (c) Ni.

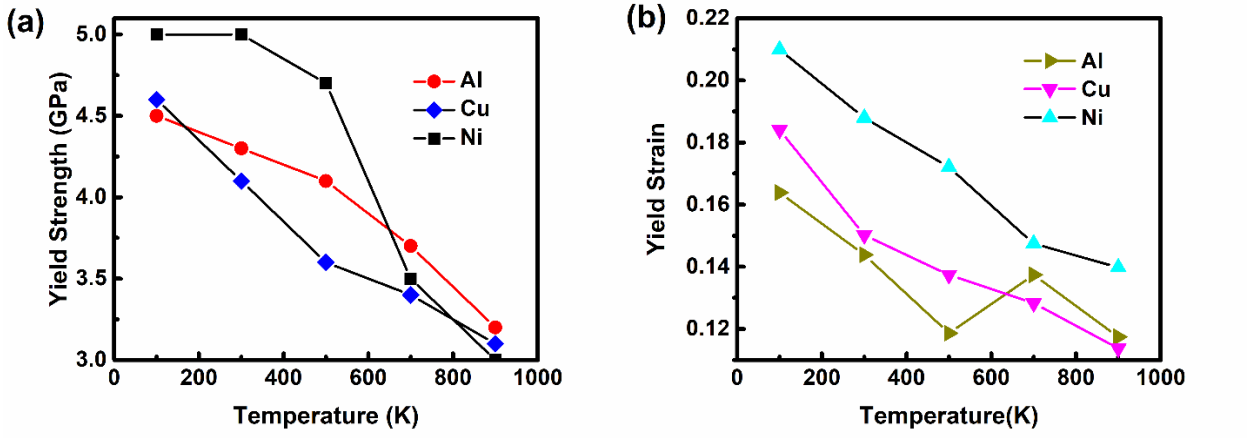

Figure 4. The Yield strength and yield strain as a function of temperature.

the transition from reversibility to irreversibility behavior of the crystals. The corresponding strain to the maximum stress was taken as the yield strain. Figure 4 shows the yield strength and strain at various temperatures. The yield strength (Figure 4a) and yield strain (Figure 4b) curves both showed a decreasing trend as temperature increased.

The yield strengths are quite high at low temperatures, showing that the atoms are well-ordered and form a compact solid crystal structure. The height of the yield strength gradually decreases as the temperature increases. This is because at higher temperatures, atoms have more oscillations, resulting in an unstable crystal structure and reduced resistance to plastic deformation. At high temperatures, atoms move relatively fast around their equilibrium location, allowing plastic flow to easily occur. The yield strain for the various temperatures employed in this study is shown in Figure 4b. Because the strain is smaller at higher temperatures, the materials yield more easily than at lower temperatures. This is due to the increased degree of structural alterations seen at high temperatures. When comparing the maximum stress in Figures. 3(a), 3(b), and 3(c), it can be seen that the stress was higher in the order of Al-Cu-Ni for the same strain. Aluminum is a very ductile material that can stretch a long way. As one moves from Al-Cu-Ni, the quantity of extension diminishes. These findings show that stresses at the nanoscale correspond to the temperature effects of plasticity observed in macro-scale experiments.

4. Conclusion

Atomistic MD simulations of uniaxial tension were performed at a constant rate of loading rate of 500 ms^{-1} on some single-crystal face centered cubic metals (Al, Cu, and Ni), to investigate the nature of deformation in these materials under different temperatures. The microstructure evolution of the crystals were analyzed. In the early stages

of loading, a significant disorder of atoms was found, resulting in elastic deformation. With a higher temperature, the reorganization of structural atoms stretched across the full length of the crystals, resulting in plastic deformation. The stress–strain diagrams obtained from the MD simulation of the tensile specimens show a rapid increase in stress up to the maximum value, followed by a sharp drop when the crystals fail due to ductile fracture. Temperature had significant effect on the yield strength. The higher the temperature, the lower the yield strength. The present results shed some light on the understanding of the mechanical properties of the nano-crystals in the MEMS and NEMS systems.

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References

[1] H. Li, K. Chandrashekhara, S. Komaragiri, S. N. Lekakh, & V. L. Richards, "Crack prediction using nonlinear finite element analysis during pattern removal in investment casting process", Journal of Materials Processing Technology **214** (2014) 1418.
[2] P. Boutachkov, K. O. Voss, K. Lee, M. S. Song, C. Yi, M. Cappellazzo, W. Kondziołka, A. Liskowicz & M. Cholewa, "An investigation of secondary electron emission from ZnO based nanomaterials for future applications in radiation detectors", Scientific Reports **11** (2021) 737.
[3] M. H. Wang, S. Y. You, F. N. Wang & Q. Liu, "Effect of dynamic adjustment of diamond tools on nano-cutting behavior of single-crystal silicon", Applied Physics A **125** (2019) 176.
[4] W. C. Crone, *A brief introduction to MEMS and NEMS*, in: W. N. Sharpe (Ed.), Springer Handbook of Experimental Solid Mechanics, Springer US, Boston, MA (2008) 203.
[5] M. S. Bobji, C. S. Ramanujan, J. B. Pethica & B. J. Inkson, "A miniaturized TEM nanoindenter for studying material deformationin situ", Measurement Science and Technology **17** (2006) 1324.
[6] E. V. Jelenković & S. To, "Suppression of nanoindentation-induced phase transformation in crystalline silicon implanted with hydrogen", Electronic Materials Letters **13** (2017) 393.
[7] D. C. Rapaport, *The art of molecular dynamics simulation*, Cambridge University Press, Cambridge (2004).
[8] T. A. Pham, K. E. Kweon, A. Samanta, V. Lordi & J. E. Pask, "Solvation and dynamics of sodium and potassium in ethylene carbonate from ab initio molecular dynamics simulations", The Journal of Physical Chemistry C **121** (2017) 21913.
[9] M. A. Pacheco-Blas & L. Vicente, "Molecular dynamics simulation of removal of heavy metals with sodium dodecyl sulfate micelle in water", Colloids and Surfaces A: Physicochemical and Engineering Aspects **578** (2019) 123613.
[10] H. Eslami, F. Mozaffari & J. Moghadasi, "Molecular dynamics simulation of potassium along the liquid-vapor coexistence curve", Journal of the Iranian Chemical Society **7** (2010) 308.
[11] D. K. Belashchenko, "Molecular dynamics simulation of the structure and thermodynamic properties of liquid rubidium at pressures of up to 10 *GPa* and temperatures of up to 3500 *K*", Russian Journal of Physical Chemistry A **90** (2016) 1707.
[12] M. Faruq, A. Villesuzanne & G. Shao, "Molecular-dynamics simulations of binary Pd-Si metal alloys: Glass formation, crystallisation and cluster properties", Journal of Non-Crystalline Solids **487** (2018) 72.
[13] K. Saitoh, K. Kuramitsu, T. Sato, M. Takuma & Y. Takahashi, "Molecular dynamics study on deformation mechanism of grain boundaries in magnesium crystal: based on coincidence site lattice theory", Journal of Materials **2018** (2018) 4153464.
[14] S. P. Patil & Y. Heider, "A review on brittle fracture nanomechanics by all-atom simulations", Nanomaterials (Basel) **9** (2019) 1050.
[15] Y. Zhang, S. Jiang, X. Zhu & Y. Zhao, "Mechanisms of crack propagation in nanoscale single crystal, bicrystal and tricrystal nickels based on molecular dynamics simulation", Results in Physics **7** (2017) 1722.
[16] P. Heino, H. Häkkinen & K. Kaski, "Molecular-dynamics study of copper with defects under strain", Physical Review B **58** (1998) 641.
[17] X. Zhao, C. Lu, A. K. Tieu, L. Pei, L. Zhang, L. Su & L. Zhan, "Deformation mechanisms in nanotwinned copper by molecular dynamics simulation", Materials Science and Engineering: A **687** (2017) 343.
[18] L. Chang, C. Y. Zhou, L. L. Wen, J. Li & X. H. He, "Molecular dynamics study of strain rate effects on tensile behavior of single crystal titanium nanowire", Computational Materials Science **128** (2017) 348.
[19] L. Chang, C. Y. Zhou, H.-X. Liu, J. Li & X. H. He, "Orientation and strain rate dependent tensile behavior of single crystal titanium nanowires by molecular dynamics simulations", Journal of Materials Science & Technology **34** (2018) 864.
[20] R. Komanduri, N. Chandrasekaran & L. M. Raff, "Molecular dynamics (MD) simulation of uniaxial tension of some single-crystal cubic metals at nanolevel", International Journal of Mechanical Sciences **43** (2001) 2237.
[21] Y. Rosandi, H.-T. Luu, H. M. Urbassek & N. Gunkelmann, "Molecular dynamics simulations of the mechanical behavior of alumina coated aluminum nanowires under tension and compression", RSC Advances **10** (2020) 14353.
[22] H. Liang, M. Upmanyu & H. Huang, "Size-dependent elasticity of nanowires: nonlinear effects", Physical Review B **71** (2005) 241403.
[23] L. Yuan, D. Shan & B. Guo, "Molecular dynamics simulation of tensile deformation of nano-single crystal aluminum", Journal of Materials Processing Technology **184** (2007) 1.
[24] P. T. Li, Y.Q. Yang, Z. Xia, X. Luo, N. Jin, Y. Gao & G. Liu, "Molecular dynamic simulation of nanocrystal formation and tensile deformation of TiAl alloy", RSC Advances **7** (2017) 48315.
[25] M. S. Daw S. M. Foiles, & M. I. Baskes, "The embedded-atom method: a review of theory and applications", Materials Science Reports **9** (1993) 251.

[26] M. S. Daw & M. I. Baskes, "Semiempirical, quantum mechanical calculation of hydrogen embrittlement in metals", Physical review letters **50** (1983) 1285.
[27] M. S. Daw, "Model of metallic cohesion: The embedded-atom method", Physical Review B **39** (1989) 7441.
[28] Q. Spreiter & M. Walter, "Classical molecular dynamics simulation with the velocity verlet algorithm at strong external magnetic fields", Journal of Computational Physics **152** (1999) 102.
[29] H. Gould & J. Tobochnik, *Statistical and thermal physics: with computer applications*, Princeton University Press (2010).
[30] P. Thompson A, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. in 't Veld, A. Kohlmeye, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott & S. J. Plimpton, "LAMMPS-a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales", Comp. Phys. Comm. **271** (2022) 108171.
[31] A. Stukowski, "Visualization and analysis of atomistic simulation data with OVITO-the open visualization tool", Modelling and Simulation in Materials Science and Engineering **18** (2010) 015012.
[32] Y. Zhao & Y. Gu, "Deformation mechanisms and plasticity of ultrafine-grained Al under complex stress state revealed by digital image correlation technique", Nanotechnology Reviews **10** (2021) 73.
[33] L. Li & M. Han, "Molecular dynamics simulations on tensile behaviors of single-crystal bcc Fe nanowire: effects of strain rates and thermal environment", Applied Physics A **123** (2017) 450.
[34] L. Pastor-Abia, M. J. Caturla, E. SanFabián, G. Chiappe & E. Louis, "Abnormal stress drop at the yield point of aluminum nanowires: A molecular dynamics study", Physical Review B **83** (2011) 165441.