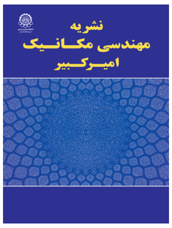

Amirkabir Journal of Mechanical Engineering

Amirkabir J. Mech. Eng., 54(2) (2022) 89-92
DOI: 10.22060/mej.2022.19779.7108

Investigation of Mechanical Behavior of Boron Nitride Nanotubes -Reinforced Magnesium Nanocomposite Using Molecular Dynamics Simulations

M. Zolfaghari[1], Y. Jafarkalhori[1], H. Heydari[2], V. Tahmasbi[3], M. Safari[3]

[1] D1 Department of Mechanic Engineering, Arak University, Arak, Iran
[2] Department of Mechanic Engineering, Shahrekord University, Shahrekord, Iran
[3] Department of Mechanic Engineering, Arak University of Technology, Arak, Iran

ABSTRACT: Magnesium-based nanocomposites are widely used in the aerospace, automotive, and medical industries. Due to the special properties of boron nitride nanotubes, these nanotubes play an important role in strengthening nanocomposites. In this research, magnesium nanocomposites are reinforced by boron nitride nanotubes and the mechanical properties of these nanocomposites under uniaxial tensile loading in the axial direction of the nanotubes have been investigated by the molecular dynamics method by Lammps software. Also, the coefficients of the atomic potential function of magnesium atoms have been calculated using the law of composition and the data extracted by Gaussian software. The results of molecular dynamics simulations show the improvement of mechanical properties of magnesium-based metal nanocomposites due to the addition of boron nitride nanotubes. The presence of boron nitride (0,12), (0,14), (0,16) and (0,18) nanotube reinforcers as magnesium field reinforcers increased the elastic modulus by 13, 14.9, 16.2 and 17 percent. Other results of this study indicate that the elastic behavior of nanocomposites is independent of strain rate changes. Also, by performing this simulation over a wide range of temperatures, obvious changes in the mechanical properties of the nanocomposite at different temperatures have been obtained.

Review History:

Received: Mar. 22, 2021
Revised: Oct. 29, 2021
Accepted: Jan. 01, 2022
Available Online: Jan. 12, 2022

Keywords:

Molecular Dynamics
Nanocomposite
Magnesium
Boron Nitride Nanotube.

1- Introduction

Magnesium, as the least dense industrial metal, has a high specific strength. Magnesium-based metal matrix nanocomposites are an important issue in the development of lightweight structural materials, as their optimized properties are critical to the automotive and aerospace industries.[1] In addition, magnesium and some of its alloys have received widespread medical attention because of their lower biodegradability and elasticity, which are closer to the natural bone than current metal implants such as titanium and its alloys, stainless steels [2]. With the discovery of Boron Nitride Nanotubes (BNNT) and its comparison with carbon nanotubes, which led to the superiority of boron nitride nanotubes, it was used as a reinforcing phase in nanocomposites [3]. In a study by Rahmat et al. [4], The shear and tensile mechanical properties of epoxy-boron nitride composite thin film were investigated and it was found that with increasing strain rate, the tensile strength and Young's modulus increased by 39% and 113%, respectively. Zhou et al. [5] simulated the molecular dynamics of the tensile test of a magnesium-based composite reinforced by a nickel-coated carbon nanotube at different temperatures and strain rates. The results showed that nickel-coated carbon nanotubes effectively improve the mechanical properties of the composite.

In the present study, due to the biocompatibility of boron-nitride nanotubes [6], the mechanical properties of magnesium-boron nitride nanocomposite, which is especially useful for orthopedic applications including implants [7], due to changes in nanotube diameter, Strain rate, and temperature are studied by molecular dynamics.

2- Methodology

In the present study, simulation by molecular dynamics method was performed using Lammps software. The present simulation requires inter-atomic potential functions of magnesium-magnesium, magnesium-boron, magnesium-nitrogen, and boron-nitrogen atoms. The Tersoff potential function is used to describe the interatomic potential of boron and nitrogen atoms. The embedded-atom method is used to describe the interaction between magnesium-magnesium particles, and the Lennard-Jones potential function is used to describe the interaction between magnesium-boron and nitrogen atoms.

The matrix model is made as a rectangular cube of magnesium atoms with an hcp structure and with lattice constants of 3.2, 3.2, and 5.2 in three directions x, y, and z by the Atomsk. The dimensions of this cube in three directions x, y, and z are 57.6, 55.43, and 83.2 angstrom, respectively, which contains 1520 magnesium atoms. Zigzag (12,0), (14,0), (16,0), and (18,0) boron nitride boron nanotubes are generated by Visual Molecular Dynamics (VMD) software.

*Corresponding author's email: hami

After modeling pure magnesium and nanotubes, it will be completed by cutting a cylindrical volume from inside the matrix and placing the nanotubes in the nanocomposite model under study. Using Lammps software, periodic boundary conditions in all three directions x, y, and z are considered for the model. Before applying the uniaxial tensile load, the energy minimization operation will be applied in one-hundred Pico-seconds with a time step of one femto-second. Using the Gaussian distribution function, the initial velocity will be given to the system and then the constructed model will be rested to balance the thermodynamic properties of the system, which requires the application of a constant pressure-constant temperature NPT at 300 K and at external pressure it is zero by the Nose-Hoover thermostat.

After releasing the sample, a load in the z-direction is applied to it at a specified strain rate of 109 s-1 [10] and the Verlet algorithm is used to integrate the Newtonian equations of classical motion equations. In this study, the simulation temperature is controlled by the NVT constant temperature canonical ensemble at 300 K and the simulation is performed in a time step of one femtosecond. During the simulation, the stress is calculated from the viral stress relation.

3- Results and Discussion

The results of stress-strain simulations show that there are four parts during the tension of the models: Primary elastic deformation in which the stress increases linearly with increasing strain. A nonlinear short elastic region and an ever-decreasing stress phase, when the stress is maximized due to the germination of defects, and a stress flow phase is caused by the interaction of defects. In other words, in these diagrams, the specimen is first stretched elastically and then its plastic deformation begins at the point of yield with the formation and dispersion of the propagation dislocation particles. The first peak point in the stress-strain diagram shows the yield point of matter as well as the first atomic dislocation within matter. The rest of the peaks in the plastic range from the stress-strain diagrams and the sudden collapse after them show the formation and propagation of the dislocations under the applied load. The increase of stress after each peak reveals the material's resistance to subsequent plastic deformation. The first peak point indicates the yield of the matrix to the applied load. The endpoint also shows the failure of the nanotube under the applied strain load. The oscillations between these two points also express the process of plastic deformation of the matrix. The general behavior of the stress-strain diagram and the peak points of this research are in good agreement with similar previous articles, so that the stress-strain diagram for aluminum-boron nitride nanocomposites, whose nanotube is an armchair type [8], has the highest initial peak point of about 7 GB. It also has several similar points that indicate an increase in the collision and interaction of these dislocations and then their release at each stage, which will lead to the creation of peak points. Also, the general behavior of the stress-strain diagram and the peak points of the present study show a good agreement with another study, which investigated aluminum nanocomposites-boron -nitride-carbon nanofibers [9].

3- 1- Effects of nanotube diameter

As the diameter of boron nitride nanotubes increases, the elastic modulus, maximum stress, and fracture stress increase significantly. However, the fracture strain in reinforced nanocomposites increases with the increasing diameter of boron nitride nanotubes. This is because the tensile stress in nanotubes is diameter dependent [10] and the magnesium-boron nitride nanotube-dominated composite is dominated by the reinforcing boron nitride nanotubes. While the failure behavior of magnesium-boron-nitride nanotubes may be controlled by more factors such as boron nitride nanotube size characteristics and deformation mechanisms. It can also be concluded that in a magnesium composite reinforced with boron nitride nanotubes, their fracture toughness increases because these nanotubes cause the failure of the composite to occur gradually.

3- 2- Effects of strain rate

The stress-strain curves at the rates of different strains in the linear elastic stage are exactly the same during tensile loading, This indicates that no apparent change in young's modulus of the composites occurs with increasing strain rate. This can be attributed to the low sensitivity of the elastic modulus to the strain rate in nanomaterials [11]. Changes in strain rate, maximum stress, and related tensile strain affect the magnesium-boron nitride nanotube composite. The energy required to overcome the dislocations over the obstacles they encounter during slip determines the dependence of the stress on the strain rate [12]. Increasing the strain rate delays the beginning of Nucleation and propagation, thereby increasing the flow stress and strain associated with it. As the atomic mobility increases due to the increase in strain rate, the chance of dislocations for propagation and interaction will decrease, and as a result, the density of the dislocation lines will increase, which will lead to an increase in flow stress with increasing strain rate. For example, at a strain rate of 0.05 (ps)-1, due to high atomic mobility, the dislocations have less chance of colliding and interacting, forming only one peak. However, at lower strain rates, this trend is less pronounced, for example, at a strain rate of 0.0001 (ps)-1, in addition to reducing the maximum stress, at this rate the chance of collisions and interactions dislocations is greater and more peaks are created.

3- 3- Effects of temperature

To investigate the effect of temperature, tensile tests were again performed on a modeled sample of magnesium-boron nitride (0,12) composite nanotubes at different temperatures in a wide range from 100 to 500K. In each of these experiments, the system temperature is controlled using a Nose-Hoover thermostat by applying an NVT constant temperature canonical ensemble to the system. The sample is subjected to a tensile load at a specified strain rate of 109 s-1. Then, the stress-strain diagram is drawn using the data obtained from the simulations. For each tensile load, the maximum stress and tensile strength decrease significantly with increasing temperature from room temperature to higher temperature, while increasing with decreasing temperature. At higher temperatures, the material exhibits softer behavior and less resistance to applied strain loads due to increased kinetic energy and particle mobility. At lower temperatures, however, kinetic energy plays a lesser role in the mobility of the particles, and the available potential energy holds them tightly together, leaving more resistance to applied strain energies. The Poisson ratio, in reverse, decreases with increasing temperature and increases with decreasing temperature. As the temperature increases, the atoms have higher kinetic energy and the material will behave softer, As a result, it will be easier to pull by applying force in the direction of tension, and it will contract more easily in the direction perpendicular to the load. That is, in exchange for axial strain, more transverse deformation occurs in the material. But at low temperatures, the opposite happens.

4- Conclusion

After performing the desired simulations and examining them, it can be concluded that the presence of boron nitride nanotube reinforcement (0,12) increases the elastic modulus by 13%, boron nitride nanotube (0,14) increases the elastic modulus by 14.9%, boron Nitride (0,16) increased the elastic modulus by 16.2% and boron nitride (0,18) nanotubes increased the elastic modulus by 17%. Also, the presence of boron nitride nanotube reinforcer significantly increases the stiffness, strength, and toughness of magnesium-boron nitride nanocomposite. In other results, with increasing temperature, maximum stress and fracture strain of magnesium-boron nitride composite nanotubes decrease except fracture stress. At higher temperatures, the material exhibits softer behavior and less resistance to applied strain loads due to increased kinetic energy and particle mobility. Young's modulus and yield strength are almost unchanged with increasing external loading rate. The change in strain rate affects the maximum stress, the corresponding tensile strain, the fracture stress, and the fracture strain of the magnesium-boron nitride composite nanotube. Also, with increasing the diameter of boron nitride nanotubes, the maximum stress and fracture stress increase significantly.

References

[1] D.K. Rajak, D.D. Pagar, R. Kumar, C.I. Pruncu, Recent progress of reinforcement materials: A comprehensive overview of composite materials, Journal of Materials Research and Technology, 8(6) (2019) 6354-6374.

[2] M. Shahin, K. Munir, C. Wen, Y. Li, Magnesium matrix nanocomposites for orthopedic applications: a review from mechanical, corrosion, and biological perspectives, Acta biomaterialia, 96 (2019) 1-19.

[3] M. Santosh, P.K. Maiti, A. Sood, Elastic properties of boron nitride nanotubes and their comparison with carbon nanotubes, Journal of nanoscience and nanotechnology, 9(9) (2009) 5425-5430.

[4] M. Rahmat, A. Naftel, B. Ashrafi, M.B. Jakubinek, Y. Martinez-Rubi, B. Simard, Dynamic mechanical characterization of boron nitride nanotube—epoxy nanocomposites, Polymer Composites, 40(6) (2019) 2119-2131.

[5] X. Zhou, X. Liu, F. Sansoz, M. Shen, Molecular dynamics simulation on temperature and stain rate-dependent tensile response and failure behavior of Ni-coated CNT/Mg composites, Applied Physics A, 124(7) (2018) 1-11.

[6] G.G. Genchi, G. Ciofani, Bioapplications of boron nitride nanotubes, in, Future Medicine, 2015, pp. 3315-3319.

[7] W. Qin, A. Kolooshani, A. Kolahdooz, S. Saber-Samandari, S. Khazaei, A. Khandan, F. Ren, D. Toghraie, Coating the magnesium implants with reinforced nanocomposite nanoparticles for use in orthopedic applications, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 621 (2021) 126581.

[8] Z. Cong, S. Lee, Study of mechanical behavior of BNNT-reinforced aluminum composites using molecular dynamics simulations, Composite Structures, 194 (2018) 80-86.

[9] V. Vijayaraghavan, L. Zhang, Tensile Properties of Boron Nitride-Carbon Nanosheet-Reinforced Aluminum Nanocomposites Using Molecular Dynamics Simulation, JOM, 72(6) (2020) 2305-2311.

[10] J. Xiang, L. Xie, S.A. Meguid, S. Pang, J. Yi, Y. Zhang, R. Liang, An atomic-level understanding of the strengthening mechanism of aluminum matrix composites reinforced by aligned carbon nanotubes, Computational Materials Science, 128 (2017) 359-372.

[11] Y. Zhou, M. Hu, Mechanical behaviors of nanocrystalline Cu/SiC composites: An atomistic investigation, Computational Materials Science, 129 (2017) 129-136.

[12] D. Hull, D.J. Bacon, Introduction to dislocations, Elsevier, 2011.

HOW TO CITE THIS ARTICLE

M. Zolfaghari, Y. Jafarkalhori, H. Heydari, V. Tahmasbi3, M. Safari3 , Investigation of Mechanical Behavior of Boron Nitride Nanotubes -Reinforced Magnesium Nanocomposite Using Molecular Dynamics Simulations, Amirkabir J. Mech Eng., 54(2) (2022) 89-92.

DOI: 10.22060/mej.2022.19779.7108