Journal of Simulation and Analysis of Novel Technologies in Mechanical Engineering
13 (4) (2021) 0031~0040
HTTP://JSME.IAUKHSH.AC.IR

Research article

Molecular simulation for prediction of mechanical properties of polylactic acid polymer for biotechnology applications

Amin Mansouri[1], Ali Heidari[1], Fatemeh Karimian[2], Amir Mohammad Gholami[3], Mehran Latifi[2*], Sheyda Shahriari[4**]

[1]*Department of Mechanical Engineering, Khomeinishahr Branch, Islamic Azad University, Isfahan, Iran*
[2]*Biotechnology Department, Falavarjan Branch, Islamic Azad University, Isfahan Iran*
[3]*Department of Mechanical Engineering, Najafabad Branch, Islamic Azad University, Isfahan, Iran*
[4]*Institute of Psychiatry, Psychiatry and Neuroscience, Kings College London, London, UK*

[*]latifi.research@yahoo.com, [**]sheyda.shahriarineuro@edu.uk

(Manuscript Received --- 12 Feb. 2022; Revised --- 05 Apr. 2022; Accepted --- 12 Apr. 2022)

Abstract
Development of materials for use in medicine and industries is one of the biggest challenges in research in materials science. Today, absorbable, biocompatible and biodegradable polymers have been identified to be used as alternative materials for biomedical applications. Among the biomaterials used in medical fields, polylactic acid (PLA) have been considered widely. This polymer obtained from completely renewable sources and due to their good physicochemical properties in various industries it is highly recommended. The purpose of this study was to introduce PLA mechanical properties using molecular dynamics (MDs) simulation. The special advantage of PLA over other polymers is its biodegradation, which is generally degraded by a single-step process involving a bacterial attack on the polymer itself. It is easily degraded in atmospheres with high humidity and temperatures of 50-70°C. However, at lower temperatures or lower humidity, the stability of PLA products is higher. The MD analysis indicates that the density value corresponds well to the experimental values. Based on the molecular model, the elastic modulus properties of the model were investigated. In this study, the average elastic modulus of the molecular PLA model was calculated to be about 2.2 GPa.

Keywords: Mechanical engineering; Molecular dynamic; Mechanical simulation; Elastic modulus

1- Introduction

In recent years, due to increasing environmental awareness, increasing oil prices and the challenges associated with global warming, attention to biopolymers has increased [1-4]. Because these polymers are obtained from renewable sources and their use has minimal environmental petroleum effects compared to conventional polymers. Today, these compounds are used in various fields such as physiotherapy, pharmacy, medicine, tissue engineering, food products and packaging materials. Body-compatible synthetic polymers are degradable and adsorbable. These polymers are easily converted to three-dimensional (3D) matrices with various structures [5-8]. Prominent compatibility and non-toxic nature and biodegradability are the end products of degradation of these polymers, which are the basis for their use in areas related to human health [6-9]. Synthetic polymers used for tissue engineering include poly-alpha-hydroxy esters [10-14]. The examples of poly-alpha-hydroxy-esters is polylactic acid (PLA) [15-21]. Today, these polymers are used separately or in copolymer form from this polymer [21-24]. In this article, we introduce this polymer as one of the important polymers and after describing the chemical structure and manufacturing method, we refer to their mechanical properties and physical properties using MD and its application. An extensive consumption of lactic acid and its derivatives in food, textile, pharmaceutical, cosmetic, chemical and especially polymer industries have led to many studies in recent years to produce this organic acid. In addition, lactic acid can be converted to beneficial substances such as propylene oxide, propylene glycol and ester lactate through chemical reactions [25-34]. The manufacture of PLA and acrylic biodegradable acids has also created an important market for pure lactic acid. PLA is a linear aliphatic thermoplastic polyester that can be extracted %۱۰۰ from renewable sources such as corn. Today, this polymer is widely used in packaging, textiles and plastic containers [35-38]. PLA belongs to the family of aliphatic polyesters, which are usually made from alpha-hydroxy acids. PLA is a thermoplastic with high strength and modulus which its raw material is produced from renewable sources such as potatoes and corn. Subsequently, major advances in process technology coupled with the reduction in the price of biologically produced lactic acid led to the commercial production of biodegradable lactic acid polymers in non-medical applications. This integration into biotechnology and chemistry was an important strategy that improved many processes in the following years. There are two chemical methods for converting lactic acid to high molecular weight PLA. Toatsu et al. was able to convert lactic acid directly into high molecular weight PLA in a basic solvent process with azeotropic removal of water by distillation [25-36]. PLA is one of the few polymers whose molecular structure can be controlled by the ratio of L and D isomers to obtain a high-weight crystalline or amorphous polymer. PLA is known as a food safety agent and can come into contact with food. This polymer decomposes without the need for a catalyst by hydrolysis of ester bonds. The rate of decomposition depends on the shape and size of the polymer object, the isomer ratio and the hydrolysis temperature [37-44]. PLA a crystalline substance with a regular chain structure; Poly L is lactic acid (PLLA), which is a heme crystal, and so with a regular chain structure; Lactic Side Poly DL (PDLLA) which is amorphous. The raw materials for the production of PLA are agricultural products such as corn, sugar beet, wheat and other products rich in starch. It is noteworthy that it is not necessary to use the main agricultural products to produce PLA, but agricultural waste can also be widely used in the production of PLA. In major industrial-to-industrial countries, due to the inclusion of agricultural waste in the production cycle of other products, there is virtually no large waste disposal to be used in the production of polylactic acid. For this reason, the raw materials needed to produce PLA in these countries are cultivated industrially. A variety of carbohydrates and nitrogenous substances have been used to produce lactic acid. The choice of raw material depends on the microstructure and the desired product. Sucrose, maltose, glucose, mannitol, etc. have been used commercially. Molasses is cheap, but has little efficiency in producing lactic acid. Corn, straw, cotton husk, etc. have also been studied [41-47]. It is vital for the agricultural industry to find profitable use for these biodegradable materials that are discarded as residual sugar extraction. This bioplastic is made from sugar beet pulp and another biodegradable polymer called PLA by extrusion process [47-51]. Whey is one of these wastes and disposables, because whey requires a great deal of biochemical oxygen, about 30,000 to 50,000 ppt, to be absorbed into nature, the amount of environmental pollution is much higher than the virtual limit set by the environmental protection agency for industrial effluents.

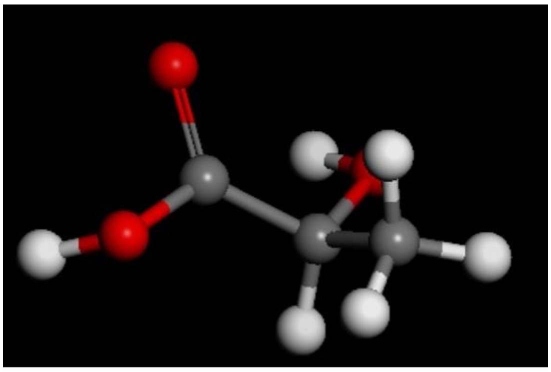

Fig. 1 Chemical structure PLA monomer using MD software

However, most of the whey from the cheese factories now enters nature in the form of waste. Interestingly, whey is more efficient than other raw materials that can be used to produce PLA. Whey has the highest production efficiency among other raw materials. However, production efficiency is not the only criterion for selecting the raw material, but the quantity and price of the raw material are the owner of the choice for industrial production. The process of producing PLA and fibers from corn is studied exclusively. In general, the production process of PLA polymer is produced in three main stages, which are conversion of corn to dextrose.

2-Chemical and physical properties of PLA

PLA is a semi-crystalline polymer with a glass transition temperature of about 55 to 59°C and a melting point of 174-184°C. It represents good mechanical strength, high elastic modulus, good thermal plasticity, good processability and this relatively hydrophobic polyester, unstable in wet conditions, which can cause chain disorders in the human body to non-toxic by-products, and lactic acid. Converts carbon and water, which is subsequently eliminated through the Krebs cycle in the urine [18]. In general, it can be said that this polymer is biocompatible, biodegradable, absorbable, semi-crystalline polymer, glass transition temperature around 55-59°C, melting point 174-184°C, high water vapor permeability, High tensile strength 50-70 MPa, low impact resistance, high hardness, thermal ductility, good processability, resistant to fat and water penetration. PLA is generally known for its good mechanical properties, with an elastic modulus of 3000-4000 MPa and tensile strength of 50-70 MPa, elongation at break point is 2-10%, flexural strength is 100 MPa and the flexural modulus is 4000-5000 MPa. Therefore, it can be an alternative to ordinary polymers in many applications, such as packaging, extrusion and heating containers [26-39]. However, there is a slight increase in length at rest, which is an example of this polymer limiting some of its applications. Fragile at room temperature, breaking through the grazing mechanism. Efforts have been made to improve the properties of PLA by copolymerization, combined with other biodegradable polymers. It should be noted that the mechanical properties of PLA do not significantly affect its synthesis methods [40-43]. It is interesting to note that material processing has a significant effect on PLA impact resistance [32-40]. Therefore, since PLA is a material characterized by a relatively low value of impact resistance, the effect of crystallization and molecular weight has been considered in scientific applications. Rockwell hardness of PLA is usually between the range of 70 and 90 according to the scale [41-47]. Rockwell hardness of PLLA is affected by very little crystallization, which for amorphous PLLA ranges from 83-88 H and 82-88H are evident for the semi-crystalline PLLA. The Rockwell hardness dependence on molecular weight also appears to be negligible. However, the effect of glass transition temperature (TG) is more pronounced. PDLLA is characterized by a lower hardness in the range of 72-78 H [41-46]. The lower hardness for PDLLA than PLLA can be explained in terms of lower triglyceride than PDLLA [48-52]. Among biodegradable polymers, PLA is characterized by high elastic modulus and high hardness. The mechanical property, which penetrates the applications of these materials, strongly depends on its chemical composition. The presence of the polar ester group in the neighborhood and its regular distribution, affect physical interactions. Finally, chain interactions between polarity and high glass temperatures are the source of high PLA hardness.

3-MDs of polylactic acid

Molecular dynamics (MDs) method is one of the numerical simulation methods that is used to simulate and obtain the physical and mechanical properties of various materials, including nanomaterials and polymers [29-39]. In this method, the numerical model of atoms and molecules is made according to the interatomic forces and after equilibrium, the physical and mechanical properties of the material are extracted using statistical mechanical equations. In many studies, this method is known as a relatively accurate method for predicting the properties or factors affecting the properties of materials. In this study, molecular dynamics simulation was used to model the PLA atomic model. In this study, the COMPASS force field is used. This force field has been successfully used to predict the properties of polymer-based materials. The molecular structure of PLA monomers is shown in Fig. 1. By creating a chain structure and random distribution of PLA molecules in an amorphous cubic simulation box with periodic boundary conditions, the PLA atomic model is constructed according to Fig. 2. The initial density of the PLA model was 1 (g/cm^3). After geometry optimization and energy minimization, molecular dynamics simulation was performed using NPT at 298 K at 40 ps.

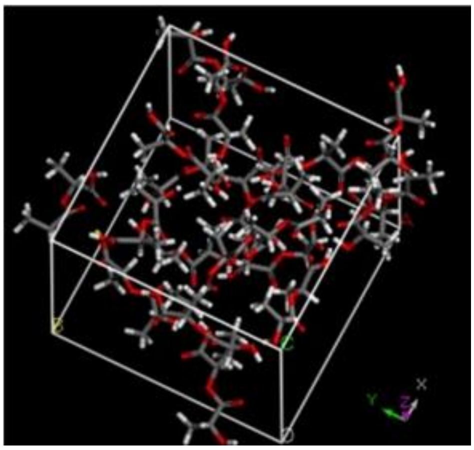

Fig. 2 Simulation box of PLA atomic model

The interaction forces of Van Der Waals and Columbus are taken into account in these calculations. The cut-off distance for atomic modeling is 12.5 A [47-52]. Fig. 3 shows the energy changes of the atomic model in the NPT simulation representing the equilibrium of the system. Fig. 4 shows the density of the molecular model in the NPT simulation converges to 1.2 (g/cm^3). This density value corresponds well to the experimental values. Based on the molecular model, the elastic properties of the model are investigated. In this study, the average elastic modulus of the molecular PLA model is calculated to be about 2.2 GPa.

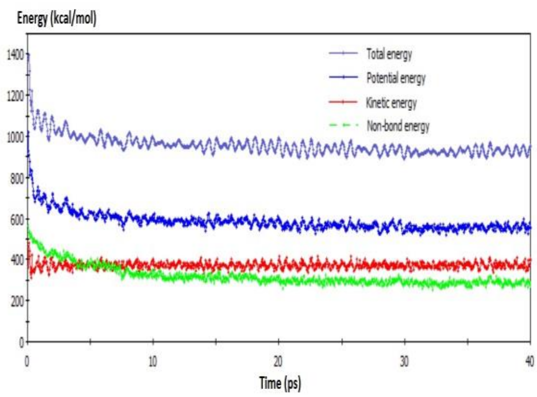

Fig. 3 Energy variations of the atomistic PLA model in NPT simulation

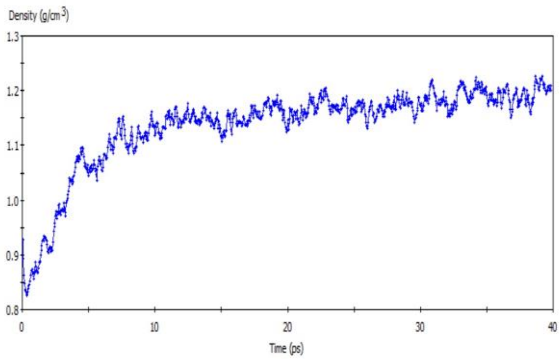

Fig. 4 Density of the atomistic PLA in NPT simulation

The main advantages of using PLA are prevention of environmental pollution, wastes from the consumption of goods made of polylactic acid are decomposed and metallized by being in the vicinity of the soil. Preventing the increase of greenhouse gases, industrial production of polylactic acid requires the cultivation of plants used as raw material on a large scale. Compatibility with living tissue, since the raw materials for the production of PLA are plants, in packaging applications, they do not transfer to packaged goods, especially food, chemicals and unnatural substances. Reducing the use of oil resources in production in the production of PLA not only is oil not used as a raw material, but its production process also requires less fuel resources. Using renewable sources, plants can be produced and recycled as raw materials for the production of PLA [41-48]. Each of these properties alone can be a strong reason for the expansion of production and use of PLA compared to today's plastics [39-52]. Despite the many advantages that PLA has over other biopolymers, its use in industry and competition with industrial polymers faces several major challenges, including crisp and brittle that needs to be improved and permeability high to water vapor and gases, low glass transition temperature

(Tg) and poor thermal stability [24, 25]. To overcome these problems can be solutions such as using suitable softeners, combining with other polymers, optimizing conditions crystallization and the use of suitable additives to produce a variety of composites. The use of nanoparticles and the production of nanocomposites to improve the properties of polymers is very important due to the great variety and effectiveness of these particles.

4-Conclusion

PLA also has non-polymeric applications, including its conversion to ethyl esters for use as natural derivatives. PLA prices will fall further as new markets for lactic acid reach new markets. PLA is first destroyed by hydrolysis, not by microbial attack. Therefore, even at high humidity, it is uncommon for high molecular weight PLAs to be contaminated by fungi, mold, or other microbes. This unusual property of the biodegradable polymer for applications where there is direct contact with food over a long period of time. This density value corresponds well to the experimental values. Based on the molecular model, the elastic properties of the model are investigated. In this study, the average elastic modulus of the molecular PLA model is calculated to be about 2.2 GPa.

References

[1] Saeedi, M. R., Morovvati, M. R., & Mollaei-Dariani, B. (2020). Experimental and numerical investigation of impact resistance of aluminum–copper cladded sheets using an energy-based damage model. Journal of the Brazilian Society of Mechanical Sciences and Engineering, 42(6), 1-24.

[2] Kardan-Halvaei, M., Morovvati, M. R., & Mollaei-Dariani, B. (2020). Crystal plasticity finite element simulation and experimental investigation of the micro-upsetting process of OFHC copper. Journal of Micromechanics and Microengineering, 30(7), 075005.

[3] Fazlollahi, M., Morovvati, M. R., & Mollaei Dariani, B. (2019). Theoretical, numerical and experimental investigation of hydro-mechanical deep drawing of steel/polymer/steel sandwich sheets. Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture, 233(5), 1529-1546.

[4] Saeedi, M. R., Morovvati, M. R., & Alizadeh-Vaghasloo, Y. (2018). Experimental and numerical study of mode-I and mixed-mode fracture of ductile U-notched functionally graded materials. International Journal of Mechanical Sciences, 144, 324-340.

[5] Morovvati, M. R., & Mollaei-Dariani, B. (2018). The formability investigation of CNT-reinforced aluminum nano-composite sheets manufactured by accumulative roll bonding. The International Journal of Advanced Manufacturing Technology, 95(9), 3523-3533.

[6] Morovvati, M. R., & Dariani, B. M. (2017). The effect of annealing on the formability of aluminum 1200 after accumulative roll bonding. Journal of Manufacturing Processes, 30, 241-254.

[7] Morovvati, M. R., Lalehpour, A., & Esmaeilzare, A. (2016). Effect of nano/micro B4C and SiC particles on fracture properties of aluminum 7075 particulate composites under chevron-notch plane strain fracture toughness test. Materials Research Express, 3(12), 125026.

[8] Fatemi, A., Morovvati, M. R., & Biglari, F. R. (2013). The effect of tube

material, microstructure, and heat treatment on process responses of tube hydroforming without axial force. The International Journal of Advanced Manufacturing Technology, 68(1), 263-276.

[9] Pourmoghadam, M. N., Esfahani, R. S., Morovvati, M. R., & Rizi, B. N. (2013). Bifurcation analysis of plastic wrinkling formation for anisotropic laminated sheets (AA2024–Polyamide–AA2024). Computational materials science, 77, 35-43.

[10] Morovvati, M. R., Fatemi, A., & Sadighi, M. (2011). Experimental and finite element investigation on wrinkling of circular single layer and two-layer sheet metals in deep drawing process. The International Journal of Advanced Manufacturing Technology, 54(1), 113-121.

[11] Morovvati, M. R., Mollaei-Dariani, B., & Haddadzadeh, M. (2010). Initial blank optimization in multilayer deep drawing process using GONNS. Journal of manufacturing science and engineering, 132(6).

[12] Fatemi, A., Biglari, F., & Morovvati, M. R. (2010). Influences of inner pressure and tube thickness on process responses of hydroforming copper tubes without axial force. Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture, 224(12), 1866-1878.

[13] Talebi, M., Abbasi-Rad, S., Malekzadeh, M., Shahgholi, M., Ardakani, A. A., Foudeh, K., & Rad, H. S. (2021). Cortical bone mechanical assessment via free water relaxometry at 3 T. Journal of Magnetic Resonance Imaging, 54(6), 1744-1751.

[14] Lucchini, R., Carnelli, D., Gastaldi, D., Shahgholi, M., Contro, R., & Vena, P. (2012). A damage model to simulate nanoindentation tests of lamellar bone at multiple penetration depth. In 6th European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS 2012 (pp. 5919-5924).

[15] Fada, R., Shahgholi, M., & Karimian, M. (2021). Improving the mechanical properties of strontium nitrate doped dicalcium phosphate cement nanoparticles for bone repair application. Ceramics International, 47(10), 14151-14159.

[16] Monfared, R. M., Ayatollahi, M. R., & Isfahani, R. B. (2018). Synergistic effects of hybrid MWCNT/nanosilica on the tensile and tribological properties of woven carbon fabric epoxy composites. Theoretical and Applied Fracture Mechanics, 96, 272-284.

[17] Ayatollahi, M. R., Barbaz Isfahani, R., & Moghimi Monfared, R. (2017). Effects of multi-walled carbon nanotube and nanosilica on tensile properties of woven carbon fabric-reinforced epoxy composites fabricated using VARIM. Journal of Composite Materials, 51(30), 4177-4188.

[18] Kamarian, S., Bodaghi, M., Isfahani, R. B., Shakeri, M., & Yas, M. H. (2021). Influence of carbon nanotubes on thermal expansion coefficient and thermal buckling of polymer composite plates: Experimental and numerical investigations. Mechanics Based Design of Structures and Machines, 49(2), 217-232.

[19] Ayatollahi, M. R., Moghimi Monfared, R., & Barbaz Isfahani, R.

(2019). Experimental investigation on tribological properties of carbon fabric composites: effects of carbon nanotubes and nano-silica. Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications, 233(5), 874-884.

[20] Kamarian, S., Bodaghi, M., Isfahani, R. B., & Song, J. I. (2020). A comparison between the effects of shape memory alloys and carbon nanotubes on the thermal buckling of laminated composite beams. Mechanics Based Design of Structures and Machines, 1-24.

[21] Barbaz-I, R. (2014). Experimental determining of the elastic modulus and strength of composites reinforced with two nanoparticles (Doctoral dissertation, Doctoral dissertation, MSc Thesis, School of Mechanical Engineering Iran University of Science and Technology, Tehran, Iran).

[22] Kamarian, S., Bodaghi, M., Isfahani, R. B., & Song, J. I. (2021). Thermal buckling analysis of sandwich plates with soft core and CNT-Reinforced composite face sheets. Journal of Sandwich Structures & Materials, 23(8), 3606-3644.

[23] Ghomi, F., Daliri, M., Godarzi, V., & Hemati, M. (2021). A novel investigation on characterization of bioactive glass cement and chitosan-gelatin membrane for jawbone tissue engineering. Journal of Nanoanalysis.

[24] Mirsasaani, S. S., Bahrami, M., & Hemati, M. (2016). Effect of Argon laser Power Density and Filler content on Physico-mechanical properties of Dental nanocomposites. Bull. Env. Pharmacol. Life Sci, 5, 28-36.

[25] Asadpoori, A., Keshavarzi, A., & Abedinzadeh, R. (2021). Parametric study of automotive shape memory alloy bumper beam subjected to low-velocity impacts. International journal of crashworthiness, 26(3), 322-327.

[26] Abedinzadeh, R. (2018). Study on the densification behavior of aluminum powders using microwave hot pressing process. The International Journal of Advanced Manufacturing Technology, 97(5), 1913-1929.

[27] Abedinzadeh, R., & Faraji Nejad, M. (2021). Effect of embedded shape memory alloy wires on the mechanical behavior of self-healing graphene-glass fiber-reinforced polymer nanocomposites. Polymer Bulletin, 78(6), 3009-3022.

[28] Abedinzadeh, R., Norouzi, E., & Toghraie, D. (2021). Experimental investigation of machinability in laser-assisted machining of aluminum-based nanocomposites. Journal of Materials Research and Technology, 15, 3481-3491.

[29] Moradi, A., Heidari, A., Amini, K., Aghadavoudi, F., & Abedinzadeh, R. (2021). Molecular modeling of Ti-6Al-4V alloy shot peening: the effects of diameter and velocity of shot particles and force field on mechanical properties and residual stress. Modelling and Simulation in Materials Science and Engineering, 29(6), 065001.

[30] Yarahmadi, A., Hashemian, M., Toghraie, D., Abedinzadeh, R., & Eftekhari, S. A. (2022). Investigation of mechanical properties of epoxy-containing Detda and Degba and graphene oxide nanosheet using molecular dynamics

simulation. Journal of Molecular Liquids, 347, 118392.

[31] Abedinzadeh, R., Shirian, H., & Parhizkar, J. (2020). Study on the Wettability and Optical Properties of Polydimethylsiloxane-SiO2 Nano-composite Surfaces. ADMT Journal, 13(4), 21-29.

[32] Abedinzadeh, R., & Gorji, R. (2017). Micromachining the Aluminium Tubes Using Abrasive Finishing in Alternating Magnetic Field. Journal of Simulation and Analysis of Novel Technologies in Mechanical Engineering, 10(4), 5-14.

[33] Abedinzadeh, R., Sattari, M., & Toghraie, D. Experimental Analysis on Bending Behavior of Non-Alloy Carbon Steel Sheets Using Laser Forming Process. steel research international.

[34] Aghadavoudi, F., Golestanian, H., & Tadi Beni, Y. (2017). Investigating the effects of resin crosslinking ratio on mechanical properties of epoxy-based nanocomposites using molecular dynamics. Polymer Composites, 38, E433-E442.

[35] Moradi-Dastjerdi, R., & Aghadavoudi, F. (2018). Static analysis of functionally graded nanocomposite sandwich plates reinforced by defected CNT. Composite Structures, 200, 839-848.

[36] Dehkordi, R. B., Toghraie, D., Hashemian, M., Aghadavoudi, F., & Akbari, M. (2021). The effects of external force and electrical field on the agglomeration of Fe3O4 nanoparticles in electroosmotic flows in microchannels using molecular dynamics simulation. International Communications in Heat and Mass Transfer, 122, 105182.

[37] Hekmatifar, M., Toghraie, D., Mehmandoust, B., Aghadavoudi, F., & Eftekhari, S. A. (2020). Molecular dynamics simulation of the phase transition process in the atomic scale for Ar/Cu nanofluid on the platinum plates. International Communications in Heat and Mass Transfer, 117, 104798.

[38] Dehkordi, R. B., Toghraie, D., Hashemian, M., Aghadavoudi, F., & Akbari, M. (2020). Molecular dynamics simulation of ferro-nanofluid flow in a microchannel in the presence of external electric field: Effects of Fe3O4 nanoparticles. International Communications in Heat and Mass Transfer, 116, 104653.

[39] Aghadavoudi, F., Golestanian, H., & Zarasvand, K. A. (2019). Elastic behaviour of hybrid cross-linked epoxy-based nanocomposite reinforced with GNP and CNT: experimental and multiscale modelling. Polymer Bulletin, 76(8), 4275-4294.

[40] Farzinpour, M., Toghraie, D., Mehmandoust, B., Aghadavoudi, F., & Karimipour, A. (2020). Molecular dynamics simulation of ferronanofluid behavior in a nanochannel in the presence of constant and time-dependent magnetic fields. Journal of Thermal Analysis and Calorimetry, 141(6), 2625-2633.

[41] Aghadavoudi, F., Golestanian, H., & Tadi Beni, Y. (2018). Investigating the effects of CNT aspect ratio and agglomeration on elastic constants of crosslinked polymer nanocomposite using multiscale modeling. Polymer Composites, 39(12), 4513-4523.

[42] Aghadavoudi, F., & Tadi Beni, Y. (2016). Investigation of cnt defects on mechanical behavior of cross linked

epoxy based nanocomposites by molecular dynamics. ADMT Journal, 9(1).

[43] Hekmatifar, M., Toghraie, D., Mehmandoust, B., Aghadavoudi, F., & Eftekhari, S. A. (2021). Molecular dynamics simulation of condensation phenomenon of nanofluid on different roughness surfaces in the presence of hydrophilic and hydrophobic structures. Journal of Molecular Liquids, 334, 116036.

[44] Moradi, A., Heidari, A., Amini, K., Aghadavoudi, F., & Abedinzadeh, R. (2021). Molecular modeling of Ti-6Al-4V alloy shot peening: the effects of diameter and velocity of shot particles and force field on mechanical properties and residual stress. Modelling and Simulation in Materials Science and Engineering, 29(6), 065001.

[45] Nasr Esfahani, M., Hashemian, M., & Aghadavoudi, F. (2022). The vibration study of a sandwich conical shell with a saturated FGP core. Scientific Reports, 12(1), 1-15.

[46] Mahale, R. S., Shamanth, V., Sharath, P. C., Shashanka, R., & Hemanth, K. (2021). A review on spark plasma sintering of duplex stainless steels. Materials Today: Proceedings, 45, 138-144.

[47] Chaudhari, V., Bodkhe, V., Deokate, S., Mali, B., & Mahale, R. (2019). Parametric optimization of TIG welding on SS 304 and MS using Taguchi approach. Int. Res. J. Eng. Technol, 6(5), 880-885.

[48] Kamble, P., & Mahale, R. (2016). Simulation and parametric study of clinched joint. Int Res J Eng Technol, 3(05), 2730-2734.

[49] Patil, A., Banapurmath, N., Hunashyal, A. M., Meti, V., & Mahale, R. (2022). Development and Performance analysis of Novel Cast AA7076-Graphene Amine-Carbon Fiber Hybrid Nanocomposites for Structural Applications. Biointerface Research in Applied Chemistry, 12(2), 1480-1489.

[50] Yadav, R. R., More, S. S., Mutekar, O. N., Mogal, A. L., & Mahale, R. S. (2019). Multilevel object sorting system using PLC controller. Int Res J Eng Technol (IRJET), 6(05), 1910.

[51] Ravishankar, S., & Mahale, R. (2015). A study on magneto rheological fluids and their applications. International Research Journal of Engineering and Technology, 2, 2023-2028.

[52] Nithin, S. K., Hemanth, K., Shamanth, V., Mahale, R. S., Sharath, P. C., & Patil, A. (2021). Importance of condition monitoring in mechanical domain. Materials Today: Proceedings.