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The 8th International Conference on Composites: Characterization, Fabrication, and Application (CCFA-8)
Dec. 20-21, 2022
Iran University of Science and Technology, Tehran, Iran

Prediction of mechanical properties of Al-C nanocomposite: a machine learning approach

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***Abstract*- Nowadays, investigating the properties of nanocomposites and finding their optimal properties pave the way for a better use of them. In this study, the main purpose is the prediction of mechanical properties of aluminum-carbon (Al-C) nanocomposite being elastic modulus and ultimate tensile stress with a machine learning algorithm. The Random Forest Regression (RFR) algorithm has been utilized in this research. Furthermore, the independent variables of T, S, and C illustrating ambient temperature, strain rate, and the content of carbon used in aluminum, respectively, and dependent variables of E and UTS indicating elastic modulus and ultimate tensile stress obtained from molecular dynamics simulation have been utilized to train the algorithm to predict the mentioned mechanical properties. The results represent that the prediction accuracies of 81.2 % and 93.1 % derived from RFR algorithm for elastic modulus and ultimate tensile stress have been obtained, respectively.**

***Keywords* -** Machine learning, Mechanical properties, Molecular dynamics, Nanocomposite

I. INTRODUCTION

Nowadays, many developments are taking place in the field of new materials such as composites [1]. Different studies are done on new composite and nanocomposite compounds. In the nano dimension, extensive studies are being conducted with new nanotechnology methods [2]. Nanocomposites are high performance materials which are a combination of unusual features and a unique design, and with an annual growth rate of about 25% they have great potential for a variety of applications [3]. Nanocomposites have practical properties. The use of nanocomposites in material processing can result in the production of single-phase or multi-phase ceramics and porous materials with special properties [4]. In recent years, due to the different mechanical properties of CNTs, carbon nanotube reinforced metal composites have attracted the attention of many scientists and researchers [5-8]. Nowadays evaluating different properties of nanomaterials is really attractive for researchers [9]. One of the most significant of properties is mechanical one. Motamedi et al. [10] investigated investigate mechanical properties of aluminum/carbon nanotubes (Al-CNT) nanocomposite and their results showed that by increasing temperature and strain rate, elastic modulus of Al-CNT nanocomposite decreases. Furthermore, the mechanical properties of aluminum/silicon nanotube were inquired by Motamedi et al. [11]. Their results indicated that by increasing the strain rate, the modulus of elasticity decreases, and no order was seen in the changing of ultimate tensile stress.

In this study, the prediction accuracy of the elastic modulus and ultimate tensile stress of aluminum/carbon (Al/C) will be discussed.

II. MODELING AND SIMULATION

MD simulation is a computational approach that can be used to study the macroscopic properties of a system by studying its microscopic properties. In order to provide the conditions for such a study, they create a situation for the atoms of that system so that these atoms can interact with each other in a certain period of time.

The equation that is solved in the molecular dynamics simulation for the atoms of the system is the Newton equation of motion. In this process, molecules and atoms are given the opportunity to interact with each other over a specified period of time. The number of components of each system is high. Therefore, numerical equations are used to determine their properties.

In this research, being used molecular dynamics simulation and LAMMPS package software, aluminum-carbon nanocomposite is tested for uniaxial tension. Periodic boundary conditions are considered for this simulation. The EAM potential [12, 13], AIREBO potential [14], and Lennard-Jones potential have been utilized to describe the

interactions between Al-Al, C-C, and Al-C atoms, respectively.

Carbon atoms are randomly distributed in the aluminum box. In this research, by using Random Forest Regression (RFR) algorithm, which is a significant algorithm in machine learning, as can be observed in TABLE I, fifteen random data have been chosen from the temperatures in the range of 300 to 900 K, the strain rates in the range of 0.001 to 0.01/ps, and the carbon contents of 2, 4, 5, and 6 %. Then the elastic modulus and ultimate tensile stress for each state have been calculated and eventually the prediction accuracy has been estimated. Meanwhile, T, S, and C are the temperature, strain rate, and carbon content, respectively, as dependent variables, and E and UTS are the elastic modulus and ultimate tensile stress, respectively, as independent variables in Table I.

TABLE I: RANDOM DATA.

T (K)	S (1/ps)	C (%)	E (GPa)	UTS (GPa)
300	0.001	2	51.074	4.68032
400	0.001	2	50.219	4.194
300	0.003	2	50.425	4.862
300	0.001	4	50.04	4.008
700	0.001	2	34.102	1.786
300	0.001	5	48.696	3.808
300	0.007	2	50.97	5.08
450	0.001	2	45.323	3.797
600	0.001	2	43.788	2.943
300	0.005	2	49.787	4.993
300	0.01	2	50.435	5.078
300	0.001	6	48.48	3.459
300	0.005	2	49.787	4.993
800	0.001	2	28.285	1.524
900	0.001	2	27.435	1.32

III. RESULTS AND DISCUSSIONS

In this part, 70 % of random data in TABLE I was used to train the Random Forest Regression algorithm, and 30 % of data was used to test to compare them with the data obtained with molecular dynamics simulation.

TABLE II indicates the results of the elastic modulus obtained from the prediction of RFR algorithm and the results obtained from molecular dynamics simulation. TABLE III indicates the results of the ultimate tensile stress obtained from the prediction of RFR algorithm and the results obtained from molecular dynamics simulation.

TABLE II: VALUES OF PREDICTED AND SIMULATED ELASTIC MODULUS.

T (K)	S (1/ps)	C (%)	Es (GPa)	Ep (GPa)
400	0.001	2	51.074	47.23874
300	0.007	2	50.97	49.99319
600	0.001	2	43.788	36.60748
300	0.005	2	49.788	50.01146
900	0.001	2	27.435	30.98116

TABLE III: VALUES OF PREDICTED AND SIMULATED ULTIMATE STRESS.

T (K)	S (1/ps)	C (%)	UTSs (GPa)	UTSp (GPa)
400	0.001	2	4.194	4.0608964
300	0.007	2	5.08	4.99751
600	0.001	2	2.943	2.4324396
300	0.005	2	4.993	4.9135792
900	0.001	2	1.32	1.9490896

Es, Ep, UTSs, and UTSp in TABLE II and TABLE III are simulated elastic modulus, predicted elastic modulus, simulated ultimate tensile stress, and predicted ultimate tensile stress, respectively. It can be found from TABLE II and TABLE III that the prediction accuracy for elastic modulus is 81.2 % (R^2 Score = 81.2 %), and prediction accuracy of ultimate tensile stress is 93.1 % (R^2 Score = 93.1 %).

IV. CONCLUSION

In this research, by using molecular dynamics simulation and RFR algorithm, the prediction accuracies of 81.2 % and 93.1 % for E and UTS of Al-C nanocomposite were obtained.

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