

Optimization of the Mechanical Properties of Al-C Nanocomposite via Response Surface Methodology: A Molecular Dynamics Study

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Abstract: Nowadays, various methods are being developed for new composites and nanocomposite compounds. Investigating the properties of nanocomposites and finding their optimal properties can enhance their utility. In this study, the mechanical molecular dynamics method was initially utilized to investigate the mechanical properties of an aluminum/carbon (Al/C) nanocomposite. Subsequently, the effect of temperature change, strain rate, and carbon content on the nanocomposite's elastic modulus and ultimate strength were investigated. To simultaneously investigate these three parameters and identify the optimal point for the elastic modulus and ultimate strength, the experimental design method for optimization was utilized. The Derringer method was utilized to determine the optimal parameters for the simultaneous optimization of two response variables, i.e., elastic modulus and ultimate strength. The findings reveal that the optimal conditions occur simultaneously at 300 K, strain rate of 0.01, and carbon content of 2 %, with an elastic modulus value of 51.046 GPa and an ultimate strength value of 5.1117 GPa. Finally, the results obtained from the RSM method were also compared with the molecular dynamics method.

Keywords: Mechanical Properties, Nanocomposites, Optimization, Response Surface Methodology

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Research paper

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1 INTRODUCTION

Numerous advancements are occurring in the field of novel materials, including composites [1]. Various research investigations are being carried out on novel composite and nanocomposite materials. In the realm of nanotechnology, there is a significant focus on conducting thorough studies utilizing innovative techniques [2]. Nanocomposites are advanced materials that possess exceptional properties due to their distinctive design and composition. With a yearly expansion rate of approximately 25%, these materials exhibit enormous potential for a diverse range of applications [3].

Nanocomposites demonstrate pragmatic characteristics. By integrating nanocomposites into material processing, it is feasible to manufacture ceramics and porous materials that are either single-phase or multi-phase and possess unique properties [4]. Over the past few years, carbon nanotube-reinforced metal composites have garnered interest from numerous researchers and scientists, owing to the distinct mechanical properties of CNTs [5-14]. In recent years, the aluminum/carbon nanotube composite has emerged as a popular topic of discussion and study within the field of metal composites [15]. Esawi et al. [16] utilized ball milling to incorporate 2 weight percent of carbon nanotubes into aluminum, resulting in a 21% rise in the tensile strength of aluminum.

Liu et al. [17] produced an aluminum/carbon nanotube composite utilizing a blend of powder metallurgy and Subsequent Friction Stir Processing (FSP). Microstructural analyses revealed that the carbon nanotubes were dispersed individually throughout the composites and had a tendency to disperse along the grain boundaries. Despite the shortening of carbon nanotubes and the formation of Al_4C_3 in the matrix, the layered structure of carbon nanotubes remained intact. Kim et al. [18] assessed the friction and wear properties of carbon nanotube composites under various conditions, such as dispersion rate, fabrication method, and carbon nanotube content. Wu et al. [19] examined the mechanical and thermal properties of aluminum/carbon nanotube composites. Using the Spark Plasma Sintering (SPS) method, they developed aluminum composites reinforced with multi-walled carbon nanotubes at concentrations ranging from 0 to 5.0 weight percent. The 0.5-weight percent multi-walled aluminum/carbon nanotube composite demonstrated a maximum thermal conductivity of 199 W/ m/ K and a maximum tensile strength of 130 MPa. These findings suggest that the multi-walled carbon nanotube aluminum matrix composite is a suitable material for high thermal conductivity applications.

Chen et al. [20] discovered that aluminum/carbon nanotube composite exhibits improved ductility with

increased tensile strength. In a separate study, Izadi et al. [21] employed a multi-pass friction stir process to generate an aluminum/multi-walled carbon nanotube composite, which exhibited double the hardness of the original alloy.

Liu et al. [22] examined the carbon nanotube shortening and strength of aluminum/carbon nanotube composites produced through multi-pass friction stir processing. The carbon nanotubes were dispersed in an aluminum matrix with a concentration of 4.5 vol. % CNT. Their analysis revealed that the change in length of carbon nanotubes has a linear relationship with the mechanical properties of the composite. Bakshi et al. [23] analyzed the tensile strength data of aluminum/carbon nanotube composites to investigate the impact of carbon nanotube dispersion and volume fraction on the elastic modulus, strength, and hardness of composites. The highest strength was observed for carbon nanotubes with a volume fraction of less than 2 vol. %. Additionally, the tensile data of magnesium/carbon nanotube and copper/carbon nanotube composites were compared with aluminum/carbon nanotube composites, revealing that reinforcement is not effective in the absence of chemical interaction between the metal matrix and the carbon nanotube.

To enhance ductility, Salama et al. [24] introduced a microstructural design of aluminum/carbon nanotube composite, revealing that dual matrix structure composites have approximately 14.8% more ductility than single matrix structure composites. The effect of carbon nanotube damage on the mechanical properties of aluminum/carbon nanotube composites was investigated by Hassan et al. [25] using damaged carbon nanotubes, which resulted in a 97.5% increase in strength and 14.2% increase in modulus compared to pure aluminum. Park et al. [26] studied the strengthening mechanisms in aluminum/carbon nanotube composites and discovered that the yield strength and tensile strength of aluminum/carbon nanotube composites improved by 60% and 23%, respectively. Due to the time-consuming and costly nature of experimental studies, molecular dynamics simulations have been utilized to predict the mechanical properties of various nanocomposites, including carbon nanotube-metal nanocomposites.

Yan et al. [27] used the molecular dynamics method to study the tensile responses of copper/carbon nanotube nanocomposites, revealing that carbon nanotubes have a significant reinforcing effect on Young's modulus and yield strength of copper/carbon nanotube nanocomposites. Motamedi et al. [28] investigated the mechanical properties of Al/CNT nanocomposites using the molecular dynamics method, as well as the continuum model of the composite and finite element method. They also employed the molecular dynamics method to predict the mechanical properties of other

nanostructures. Silvestre et al. [29] studied the compressive behavior of carbon nanotube-reinforced aluminum composites using the molecular dynamics method, revealing that Young's modulus of the composite increased by more than 60% compared to pure aluminum.

In previous studies, a large number of investigations have been conducted on aluminum-based composites; however, no significant study has been carried out on Al/C nanocomposites. Thus, in this research, first, the effect of different parameters including ambient temperature, strain rate, and carbon content utilized in the aluminum matrix have been assessed on the mechanical properties of Al/C nanocomposite. Then, the prediction and optimization of mechanical properties of Al/C nanocomposite have been fulfilled via response surface methodology.

2 SIMULATION METHOD

Molecular Dynamics (MD) simulation is a computational technique that enables the study of the macroscopic properties of a system by examining its microscopic properties. The simulation creates a scenario in which the atoms of the system interact with each other over a specified period of time. The simulation solves Newton's equation of motion for the atoms of the system, and numerical equations are used to determine their properties due to the high number of components in each system. In the present research, the aluminum-carbon nanocomposite was subjected to uniaxial tension using molecular dynamics simulation and LAMMPS package software, and periodic boundary conditions were considered ("Fig. 1").

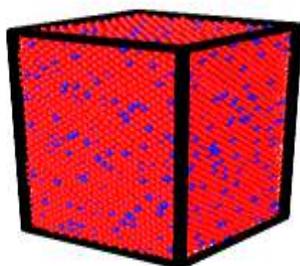


Fig. 1 Simulation box of Al-C.

The AIREBO [30-31], EAM [32], and Lennard-Jone [33] potentials were utilized to describe the interactions between C-C, Al-Al, and Al-C atoms, respectively. The aluminum-carbon nanocomposite box's dimensions were set to $80 \times 80 \times 80 \text{ \AA}^3$. The NPT ensemble was used to balance the system, with variables representing the

number of atoms, ambient pressure, and temperature. The system was found to be in perfect equilibrium with a relaxation time of 1000 ps and a time step of 1 fs. The tensile properties of the aluminum-carbon nanocomposite, including elastic modulus and ultimate tensile strength, were investigated at different temperatures of 300, 400, 450, and 600 K and strain rates of 0.001 /ps, 0.003 /ps, 0.005 /ps, 0.007 /ps, and 0.01 /ps, under ambient pressure of 100 KPa and different percentages of carbon content in the alloy, ranging from 2 % to 6 %.

3 RESULTS AND DISCUSSION

3.1. Effect of Different Parameters on the Mechanical Properties

3.1.1. Effect of Ambient Temperature

In this part, the effect of different ambient temperatures of 300, 400, 450, and 600 K has been evaluated on the mechanical properties of the Al/C nanocomposite as can be shown in "Fig. 1". The content of C used in the aluminum matrix is 2 %. Also, the Al/C nanocomposite has been simulated under uniaxial tension with a strain rate of 0.001/ps. "Table 1" shows the values of the mechanical properties derived from "Fig. 2".

Table 1 The values of the mechanical properties of Al/C nanocomposite at different ambient temperatures

Temperature, K	Elastic modulus, GPa	Ultimate tensile strength, GPa
300	51.074	4.68
400	49.655	4.194
450	46.653	3.797
600	44.942	2.943

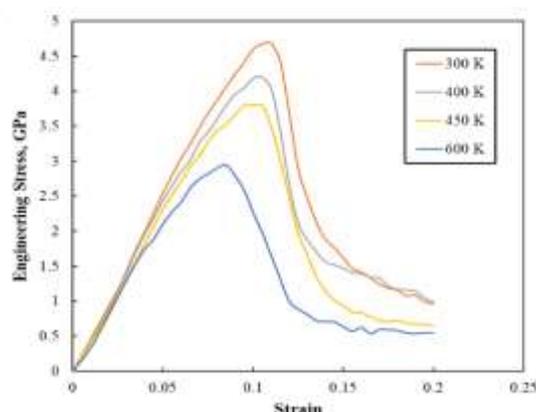


Fig. 2 Stress-strain curves of Al/C nanocomposite at different ambient temperatures.

It can be found from "Table 1" that by increasing the ambient temperature from 300 to 600 K, the elastic modulus and ultimate tensile strength have decreased by 12.006 % and 37.115 %, respectively.

3.1.2. Effect of the Strain Rate

In this subsection, the effect of different strain rates of 0.001, 0.003, 0.005, 0.007, and 0.01/ps has been evaluated on the mechanical properties of Al/C nanocomposite which has been simulated under uniaxial tension at the ambient temperature of 300 K. The carbon content used in the aluminum matrix is 2 %. Figure 3 shows the stress-strain curves at different strain rates and “Table 2” illustrates the values of obtained mechanical properties from “Fig. 3”.

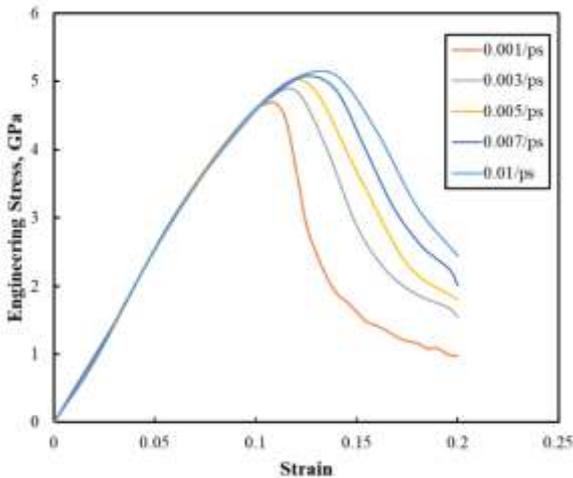


Fig. 3 Stress-strain curves of Al/C nanocomposite at different strain rates.

Table 2 The values of the mechanical properties of Al/C nanocomposite at various strain rates

Strain rate, 1/ps	Elastic modulus, GPa	Ultimate tensile strength, GPa
0.001	51.074	4.68
0.003	50.245	4.862
0.005	51.163	4.993
0.007	50.975	5.081
0.01	50.95	5.087

It can be understood from “Table 2” that by increasing the strain rate from 0.001/ps to 0.01/ps, the elastic modulus has remained constant and the ultimate tensile strength has enhanced by 8.696 %.

3.1.3. Effect of the Carbon Content

In this part, the effect of carbon content from 2 to 6 % utilized in the aluminum matrix has been assessed on the mechanical properties of Al/C nanocomposite. The nanocomposite has been simulated under uniaxial tension at the strain rate of 0.001/ps and the ambient temperature of 300 K. Figure 4 indicated stress-strain curves of Al/C nanocomposite with different carbon content and the values of the mechanical properties derived from this figure are reported in “Table 3”.

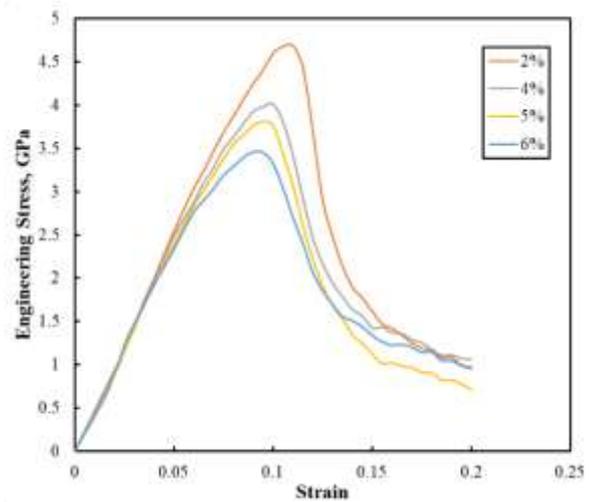


Fig. 4 Stress-strain curves of Al/C nanocomposite.

Table 3 The values of the mechanical properties of Al/C nanocomposite with different carbon content

Content, %	Elastic modulus, GPa	Ultimate tensile strength, GPa
2	51.074	4.68
4	50.392	4.008
5	48.119	3.808
6	48.087	3.459

It can be found from “Table 3” that by increasing the carbon content from 2 to 6 %, the values of elastic modulus and ultimate tensile strength have declined by 5.848 % and 26.089 %, respectively.

3.2. Statistical Modeling and Optimization

In the design of the experiment (DOE), some input parameters, which are known as independent variables, are chosen randomly. Then, some experiments or simulations are conducted to derive the results to utilize them as output parameters, which are known as dependent variables, in DOE and perform some optimizations on them. In this research, strain rate, temperature, and content of carbon utilized in the aluminum matrix are considered input variables, while the output variables are the modulus of Elasticity (E) and Ultimate Tensile Strength (UTS). Furthermore, MINITAB software has been used to execute the Response Surface Methodology (RSM) approach as a DOE method.

The Box-Behnken Design (BBD) is used as the experimentation strategy. The strain rate and temperature have been considered in 4 and 5 levels, respectively, and the number of the levels of carbon content is four, which can be observed in “Table 4”.

Table 4 The levels of input parameters

Input parameters	Levels				
Temperature, K	300	400		450	600
Strain rate, 1/ps	0.001	0.003	0.005	0.007	0.01
Content, %	2	4	5	6	

Table 5 The values of output variables

Run order	T (K)	S (1/ps)	C (%)	E (GPa)	UTS (GPa)
1	300	0.001	2	51.074	4.68
2	400	0.001	2	49.653	4.194
3	450	0.001	2	46.653	3.797
4	600	0.001	2	44.992	2.943
5	300	0.001	2	51.074	4.68
6	300	0.003	2	50.245	4.682
7	300	0.005	2	51.163	4.993
8	300	0.007	2	50.975	5.081
9	300	0.01	2	50.95	5.087
10	300	0.001	2	51.074	4.68
11	300	0.001	4	50.392	4.008
12	300	0.001	5	48.419	3.808
13	300	0.001	6	48.087	3.459
14	300	0.001	5	48.419	3.808
15	300	0.001	5	48.419	3.808

“Table 5” indicates the values of output variables for 15 simulations in different conditions. T, S, C, E, and UTS in “Table 5” show ambient temperature, strain rate, the content of carbon utilized in the aluminum matrix, elastic modulus, and ultimate tensile strength, respectively.

3.2.1. The Mathematical Modeling for Elastic Modulus

The mathematical modeling for elastic modulus is proposed by analysis of variance (ANOVA). The results of ANOVA for modulus of elasticity have been illustrated in Table 6. Furthermore, the mathematical model for elastic modulus is shown in Equation (1):

$$E = 61.86 - 0.0381 T - 144 S - 0.35 C + 12566 S*S \quad (1)$$

Where, T is the temperature in Kelvin, C is the carbon content in percent, and S is the strain rate in picoseconds. As can be observed in Equation (1), the value of E can be obtained as a function of temperature, carbon content, and strain rate. According to the analysis of variance for elastic modulus, the confidence interval is 95 % because the probability value (P-Value) in “Table 6” is remarkably less than 5 %. Moreover, the R^2 and R^2 adjusted correlation coefficients are 93.07 % and 87.87 % for elastic modulus, which show appropriate fittings for the mathematical modeling of elastic modulus proposed by the ANOVA method.

Table 6 Analysis of variance for elastic modulus

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	6	46.2788	7.7131	17.91	0.000
Linear	3	35.9790	11.9930	27.84	0.000
T	1	29.8141	29.8141	69.22	0.000
S	1	0.0021	0.0021	0.00	0.946
C	1	9.9389	9.9389	23.07	0.001
Square	3	0.3539	0.1180	0.27	0.843
T*T	1	0.2150	0.2150	0.5	0.500
S*S	1	0.0768	0.0768	0.18	0.684
C*C	1	0.0606	0.0606	0.14	0.717
Error	8	3.4458	0.4307		
Lack-of-Fit	4	3.4458	0.8615	*	*
Pure Error	4	0.0000	0.0000		
Total	14	49.7246			

$$R\text{-sq} = 93.07 \%, R\text{-sq(adj)} = 87.87 \%$$

3.2.2. The Mathematical Modeling for Ultimate Tensile Strength

In this part, the mathematical modeling for the ultimate tensile strength method has been shown as follows:

$$UTS = 6.472 - 0.00364 T + 94.1 S - 0.301 C - 4002 S*S \quad (2)$$

Where, S is the strain rate in picoseconds, T is the ambient temperature in Kelvin, C is the content of carbon in percent, and UTS is the ultimate tensile strength in GPa.

“Table 7” indicates the ANOVA results for ultimate tensile strength.

Table 7 Analysis of variance for ultimate tensile strength

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	6	5.83231	0.97205	199.37	0.000
Linear	3	3.72378	1.24126	254.59	0.000
T	1	2.29432	2.29432	470.57	0.000
S	1	0.16925	0.16925	34.74	0.000
C	1	1.19231	1.19231	244.55	0.000
Square	3	0.00998	0.00333	0.68	0.587
T*T	1	0.00319	0.00319	0.65	0.442
S*S	1	0.00778	0.00778	1.6	0.242
C*C	1	0.00002	0.00002	0.00	0.951
Error	8	0.03900	0.00488		
Lack-of-Fit	4	0.03900	0.00975	*	*
Pure Error	4	0.00000	0.00000		
Total	14	5.87132			

R-sq = 99.34 %, R-sq(adj) = 98.84 %

It can be found from “Table 7” that the probability value of ultimate tensile strength is significantly less than 5 %, and this value is desirable. In addition, for this model, the correlation coefficients of R² and R² adjusted are 99.34 % and 98.84 %, respectively, which shows the accuracy and adequacy of this model.

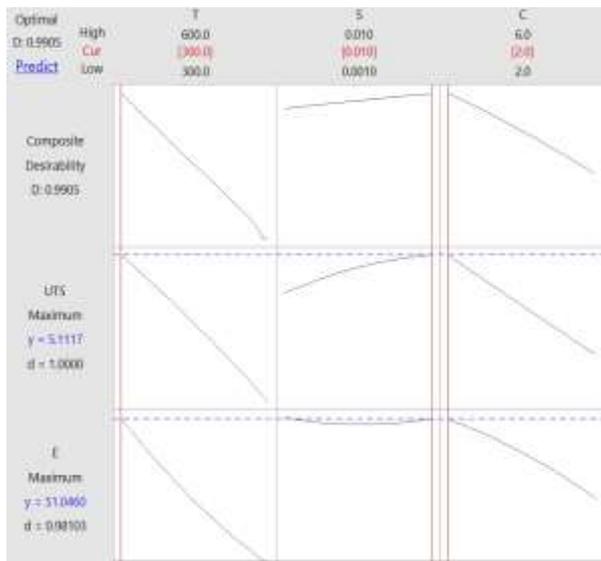


Fig. 5 The optimal values of elastic modulus and ultimate tensile strength proposed by RSM.

3.2.3. Optimization with Desirability Approach

The purpose of the optimization in this study is to maximize the values of ultimate tensile strength and modulus of elasticity by using the desirability approach. For this purpose, the results of the maximization of

elastic modulus and ultimate tensile strength are shown in “Fig 5”. It is clear in this figure that when the temperature, strain rate, and content of carbon are 300 K, 0.01/ps, and 2 %, respectively, ultimate tensile strength and elastic modulus have their maximum values. According to “Fig. 5”, the maximum predicted values of ultimate tensile strength and elastic modulus are 5.1117 GPa and 51.046 GPa, respectively. Then, in order to verify the maximum predicted values of E and UTS, the simulation in the proposed conditions (T = 300 K, S = 0.01/ps, and C = 2 %) has been simulated, which can be seen in “Fig. 6”. In this figure, the values of elastic modulus and ultimate tensile strength are 50.95 GPa and 5.087 GPa, respectively. The accuracy of the predicted and simulated value of elastic modulus is 99.811 %, also 99.514 % for ultimate tensile strength, which shows that the proposed model is profoundly desirable.

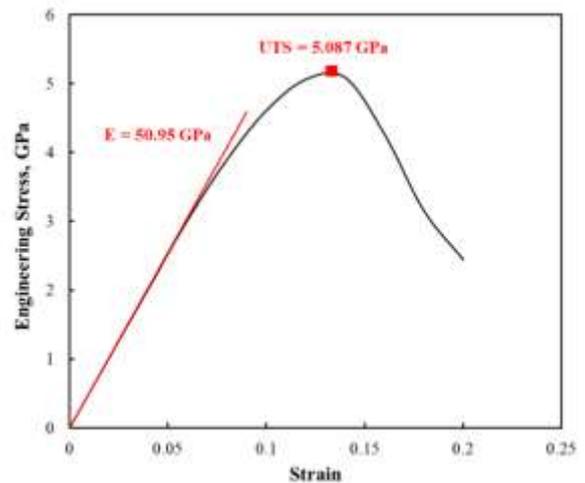


Fig. 6 Stress-strain curve of Al-Cu alloy for the proposed model.

4 CONCLUSIONS

In this study, first, the effect of ambient temperature, strain rate, and carbon content used in the aluminum matrix have been investigated on the mechanical properties of Al/C nanocomposite. The results showed that by increasing the temperature from 300 to 600 K, the elastic modulus and ultimate tensile strength decreased by 12.006 % and 37.115 %, respectively. Furthermore, by enhancing the strain rate from 0.001/ps to 0.01/ps, the E remained constant and UTS grew by 8.696 %. Moreover, the higher the carbon content, the lower the E and UTS. Then, some mathematical models were proposed by ANOVA for the prediction of E and UTS. Eventually, the E and UTS were simultaneously optimized through response surface methodology and validated via molecular dynamics simulation.

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