International Journal of
Nanoscience and Nanotechnology

Research Article 2025, Volume 21, Issue 1

Interfacial Properties of Aluminium Nanocomposites Reinforced with Graphene and Carbon Nanotube with and Without Defects at Different Temperatures Via Molecular Dynamics Simulation

Wijdan Qahtan Farhan Al-Humairi, Samrand Rash-Ahmadi*, Morteza Khalilian

Received 11/14/2024
Accepted 2/20/2025

DOI: 10.22034/ijnn.2025.2045755.2603

International Journal of Nanoscience and Nanotechnology

Abstract

Over the last decade, the use of aluminium nanocomposites reinforced with graphene nanoplates and carbon nanotubes has increased. Therefore, it is essential to examine the properties of the aluminium matrix in relation to the reinforcements. In this study, molecular dynamics simulation was used to investigate the interfacial properties of several layers of graphene nanosheets and carbon nanotubes (with and without defects) in aluminium nanocomposites. The effect of temperature and the number of reinforcements was investigated in this work. The results show that by increasing the number of graphene nanoplates and carbon nanotubes (1 to 4) in the aluminium matrix, the adhesion and interaction energy improved (-600 to-2800 kcal/mol) (-400 to-1500 kcal/mol). In addition, the highest amount of pull-out force of aluminium nanocomposites reinforced with graphene, corresponding to 4-layer graphene, was equal to 66 kcal/mol, and for aluminium nanocomposites reinforced with carbon nanotubes, corresponding to 4 carbon nanotubes, was equal to 61 kcal/mol. Also, defects in graphene nanoplates and carbon nanotubes reduce the interaction energy and pull-out force in aluminium nanocomposites. In addition, with the increase in temperature (300 to 450 K), the amount of interaction energy, adhesion, and the maximum pull-out force decreases.

Keywords: Interfacial Properties, Adhesion, Alumina Nanocomposites, Graphene, Molecular Dynamics

How to cite this article

Farhan Al-Humairi WQ, Rash-Ahmadi S, Khalilian M. Interfacial Properties of Aluminium Nanocomposites Reinforced with Graphene and Carbon Nanotube with and Without Defects at Different Temperatures Via Molecular Dynamics Simulation. Int. J. Nanosci. Nanotechnol., 2025;1: 41-48. DOI: 10.22034/ijnn.2025.2045755.2603

1. Introduction

Aluminium metal has been the focus of researchers due to its extraordinary properties, such as lightweight [1], high thermal conductivity [2], ease of processing [3], and hammerability [4]. However, aluminium also has weaknesses that limit its use in some industries. Such weakness is due to the low tensile strength of this metal [5, 6]. In the last decade, to improve the low tensile strength of aluminium metal, carbon reinforcements such as graphene nanoplates [7] and carbon nanotubes [8] have been used. Graphene nanoplates and carbon nanotubes are very suitable options for strengthening the aluminium matrix due to their low weight [9] and high strength [10, 11]. However, the addition of graphene sheets and carbon nanotubes to the aluminium matrix changes the overall properties of the nanocomposite. The result of investigating the properties between the aluminium matrix and carbon reinforcements is also of particular importance. Because the properties between the reinforcements and the aluminium matrix are directly related to the mechanical properties of the nanocomposite. According to previous studies, the results of Kumar's [12] molecular dynamics study show that the position of aluminium atoms on the surface of graphene has a direct effect on the interfacial properties between aluminium atoms and graphene. By changing the position of the aluminium atoms, the number of interactions between the surface of graphene and the aluminium atoms changes. In addition, the results of the study by Jiang et al. [13] showed that increasing the temperature from 150 K to 600 K reduced the maximum normal tensile stress on the surface of the aluminium matrix and graphene. The orientation of graphene and aluminium matrix has a direct effect on the mechanical properties of aluminium/ graphene nanocomposite [14]. In addition, in another molecular dynamics study, the results of Kumar et al. [15] show that the interaction between the aluminium matrix and graphene nanoflakes significantly affects the crystallization temperature of aluminium. On the other hand, the number of carbon

Department of Mechanical Engineering, Urmia University, Urmia, Iran.
E-mail: s.rashahmadi@urmia.ac.ir

nanotubes in aluminium composites reinforced with carbon nanotubes is directly related to the thickness of the interphase layer and the modulus of elasticity of the composite. Li et al. [16] in an experimental study showed that by increasing the annealing temperature of the composite, the level of bonding between the graphene sheets and the aluminium matrix improved. In addition, Li et al. [17] showed that the bonding relationship between the aluminium matrix and carbon nanotubes can directly affect the overall mechanical properties. Also, Guarda et al. [18] in a molecular dynamics study showed that porous graphene improves the surface adhesion of graphene-reinforced aluminium nanocomposites, as well as the tensile strength and surface shear strength of the nanocomposite when the aluminium is previously melted and then crystallized is higher. In this study, molecular dynamics simulation was used to investigate the effect of several layers of graphene and carbon nanotubes on the interfacial properties of interaction energy in the aluminium matrix under different temperatures. It is crucial to examine the interfacial properties (adhesion) between the aluminium matrix and the reinforcements, as enhancing this adhesion can improve the mechanical properties (such as tensile strength and Young's modulus) of nanocomposites [19]. Previous research indicates that a thorough study of the interfacial properties of aluminium nanocomposites reinforced with several graphene nanosheets and carbon nanotubes (both with and without defects) at various temperatures has not been conducted. Therefore, it is important to investigate and compare these parameters.

2. Simulation and method

2.1. Modelling of aluminium nanocomposites reinforced with Graphene and carbon nanotube

All aluminium composites reinforced with carbon nanotubes were modelled in dimensions of 30 x 30 x 30 angstroms. To prevent aluminium atoms from overlapping with graphene atoms, aluminium atoms that are less than 1.1 angstroms away from carbon atoms are removed. The distance between graphene nanoplates and carbon nanotubes in the aluminium matrix was considered equal to 2.4 Angstroms. In addition, for graphene nanosheets and carbon nanotubes, one percent of defects was considered as efficiency in their structure. Defects in nano-reinforcements were considered monovacancy defects. [20] (Figure 1). Also, these defects (Monovacancy defect) were added efficiently in the nanostructures as 1% for each graphene nanosheet or carbon nanotube. In this work, carbon nanotubes 4x4 with a length of 30 angstroms were used. Also, the armchair nanostructure with dimensions of 30 x 30 angstroms was used for graphene. Figure 1 shows the shape of a graphical representation of the modelled composites.

2.2. Force Fields

The Tersoff potential function [21] was used for the interaction between carbon atoms of graphene nanosheets and carbon nanotubes. Also, the EAM potential function was used for interactions between aluminium atoms. [22]. For aluminium nanocomposites reinforced with graphene nanoplates and carbon nanotubes, the sum of these two potential functions was used. Equation 1 shows the potential of the Tersoff potential function, and Equation 2 shows the potential of the EAM potential function.

$$E = \frac{1}{2}\sum_{i}\sum_{i\neq j} V_{ij} \quad (1)$$

E (Kcal/mol) shows the energy of the system. V_{ij} (Kcal/mol) is the binding energy (Binding energy is the minimum amount of energy needed to remove a particle from a system or to break down a system into its components).

$$E_i = F_a\left(\sum_{i\neq j}\rho_\beta\left(r_{ij}\right)\right) + \frac{1}{2}\sum_{i\neq j}\varnothing_{\alpha\beta}\left(r_{ij}\right) \quad (2)$$

where $\varnothing_{\alpha\beta}$ represents a pair-wise potential function (To calculate interactions for metal matrix using EAM method potentials), r_{ij} shows the distance between atoms i and j, ρ_β denotes how much the atom contributes to the electron charge density, and F is a function that provides the energy required to position atom i of type α in the electron cloud.

2.3. Simulation details

For the simulation of nanocomposites, the open-source code Lammps [23] was used. The unit of simulation systems was assumed to be metal. The boundary conditions for the nanocomposites were assumed to be periodic in all three dimensions. To achieve system equilibrium, the energy was minimized (minimize 1e-25 1e-25 1000 10000). The NVT ensemble (constant volume, constant temperature) was used in the simulations. The time step for the simulations was set to 0.001 picoseconds,

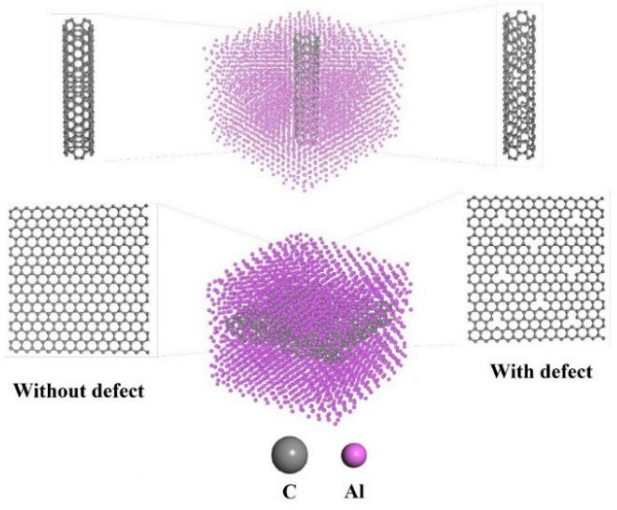

Figure 1. Graphical output of the composites modeled.

based on the simulation system's unit type. Additionally, to simulate the pulling of the nano-reinforcers from the aluminium matrix on the opposite side, a fixed and non-moving nanocomposite (fix set force) was applied to determine the pull-out force between the aluminium matrix and the nano-reinforcers. The molecular dynamics simulation algorithm converged based on the number of simulation repetitions (runs), with a total of 100 $\times 10^3$ runs conducted in this study. The simulations were also repeated several times to ensure adequate convergence.

2.4. Interaction energy

The interaction energy shows the degree of adhesion between the surface of the matrix and the carbon nanotube. The more negative the numerical value of interaction energy, the greater the amount of adhesion (interaction energy), and conversely, the more positive the numerical value of interaction energy is, the lower the amount of adhesion. Equations 3 and 4 show the interaction energy equation. [24, 25]. According to equations 3 and 4, the amount of interaction energy of the nanocomposite is equal to the potential energy of the entire nanocomposite system minus the potential energy of the aluminium matrix, and graphene nanoplates or carbon nanotubes separate. Also, Figure 2 shows the pullout simulation of the nanocomposite.

$$E_{interaction}=E_{Al/GNs}-(E_{Al}+E_{GNs}) \quad (3)$$

$$E_{interaction}=E_{Al/CNT}-(E_{Al}+E_{CNT}) \quad (4)$$

3. Results and discussion

3.1. The effect of the number of reinforcements on the interaction energy in aluminium nanocomposites

Figure 3 shows the potential energy changes of the aluminium nanocomposite reinforced with several carbon nanotubes. According to Figure 3, part a, by increasing the number of graphene nanoplates (1 to 4) in the aluminium matrix, the potential energy of the composites decreases from -12500 to -19500. Figure 3, part b, also shows the changes in the potential energy of aluminium nanocomposites reinforced with carbon nanotubes. In these graphs, the amount of potential energy decreases from -11500 to -15580 by increasing the number of carbon nanotubes from 1 to 4. The results of the diagrams in Figure 3, part b, shows that by increasing the number of reinforcements to the aluminium matrix, the amount of strong interaction energy between the aluminium matrix and carbon atoms is created. Figure 4, parts a and b, show the amount of interaction energy (adhesion) of aluminium nanocomposites reinforced with several graphene nanoplates and carbon nanotubes. According to diagrams a and b, the amount of adhesion or energy interaction increases with the increase in the number of reinforcements. According to Figure 4, graphs a and b, the highest amount of interaction energy for aluminium nanocomposites reinforced with 4 graphene layers is equal to -2800 Kcal/mol, and 4 carbon nanotubes are equal to -1500 Kcal/mol. Also, the lowest amount of interaction energy related to aluminium nanocomposites reinforced with one nanoplate of graphene is equal to -600 kcal/mol, and a carbon nanotube is -400 kcal/mol.

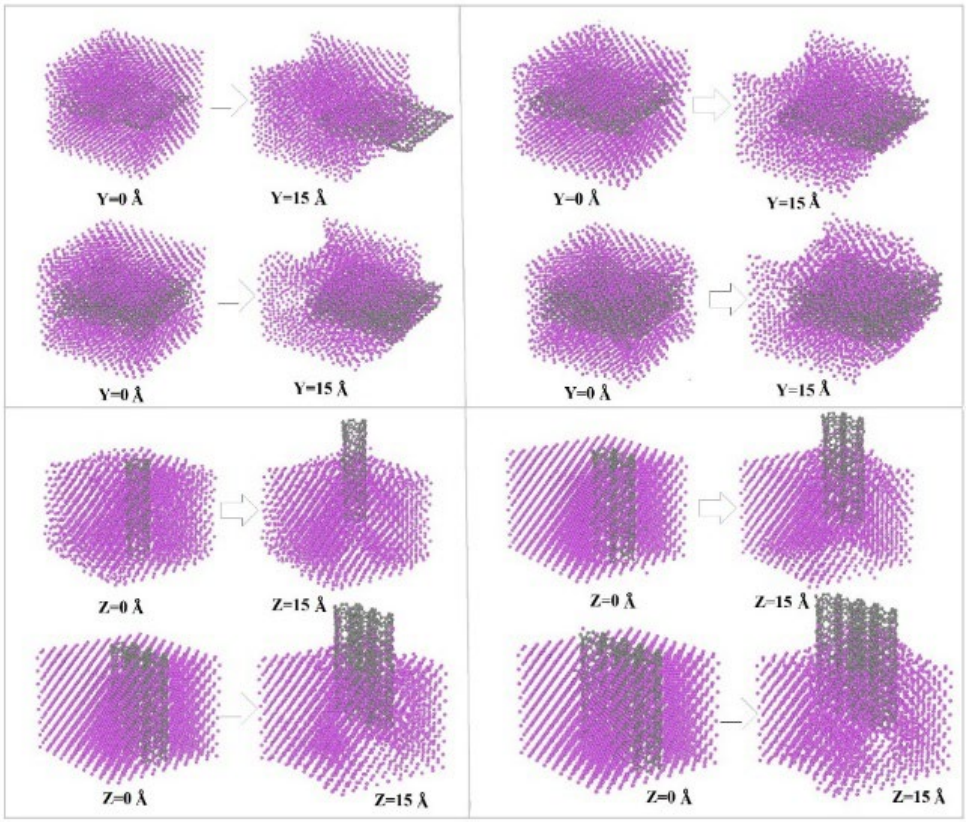

Figure 2. The pullout simulation of the nanocomposite reinforced with several carbon nanotubes and graphene.

Figure 4, in parts c and d, shows diagrams of the amount of pull-out force of aluminium nanocomposites reinforced with carbon nanotubes. According to Figure 4, part c, the highest amount of pull-out force related to aluminium nanocomposites reinforced with 4 layers of graphene nanoplate is equal to 66 kcal/mol. Also, the lowest amount of pullout force related to aluminium nanocomposites reinforced with one layer of graphene is equal to 47 kcal per mole. Also, in Figure 4, part d, the highest amount of pull-out force is related to aluminium nanocomposites reinforced with 4 carbon nanotubes, equal to 61 Kcal/mol. Also, the lowest amount of pull-out force is related to the aluminium nanocomposite reinforced with one carbon nanotube, equal to 42 Kcal/mol.

Increasing the number of nano-reinforcers in the aluminium matrix due to the increase in van der Waals and electrostatic forces between the nano-reinforcers and the aluminium matrix. Therefore, the interaction energy

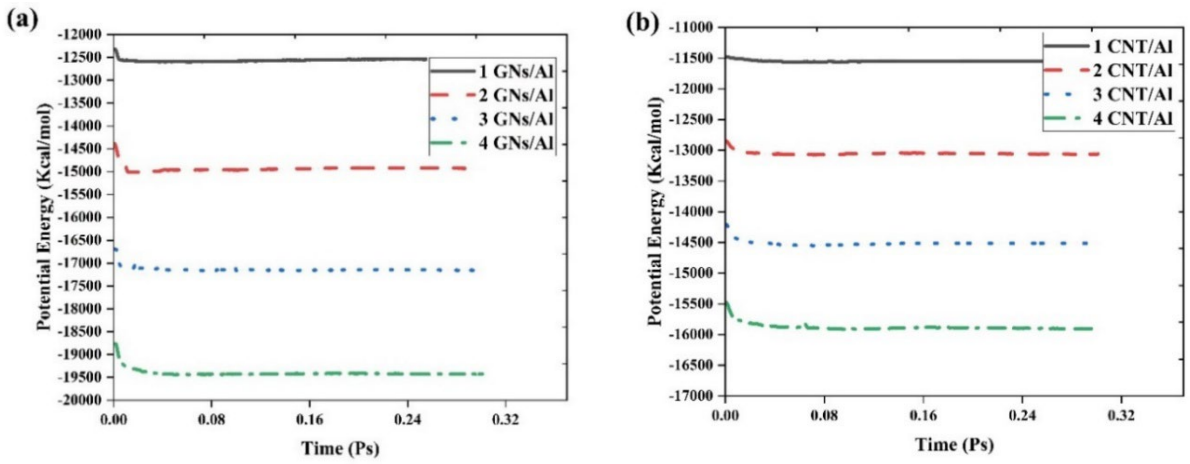

Figure 3. Potential energy changes of aluminium nanocomposite reinforced with several carbon nanotubes and graphene.

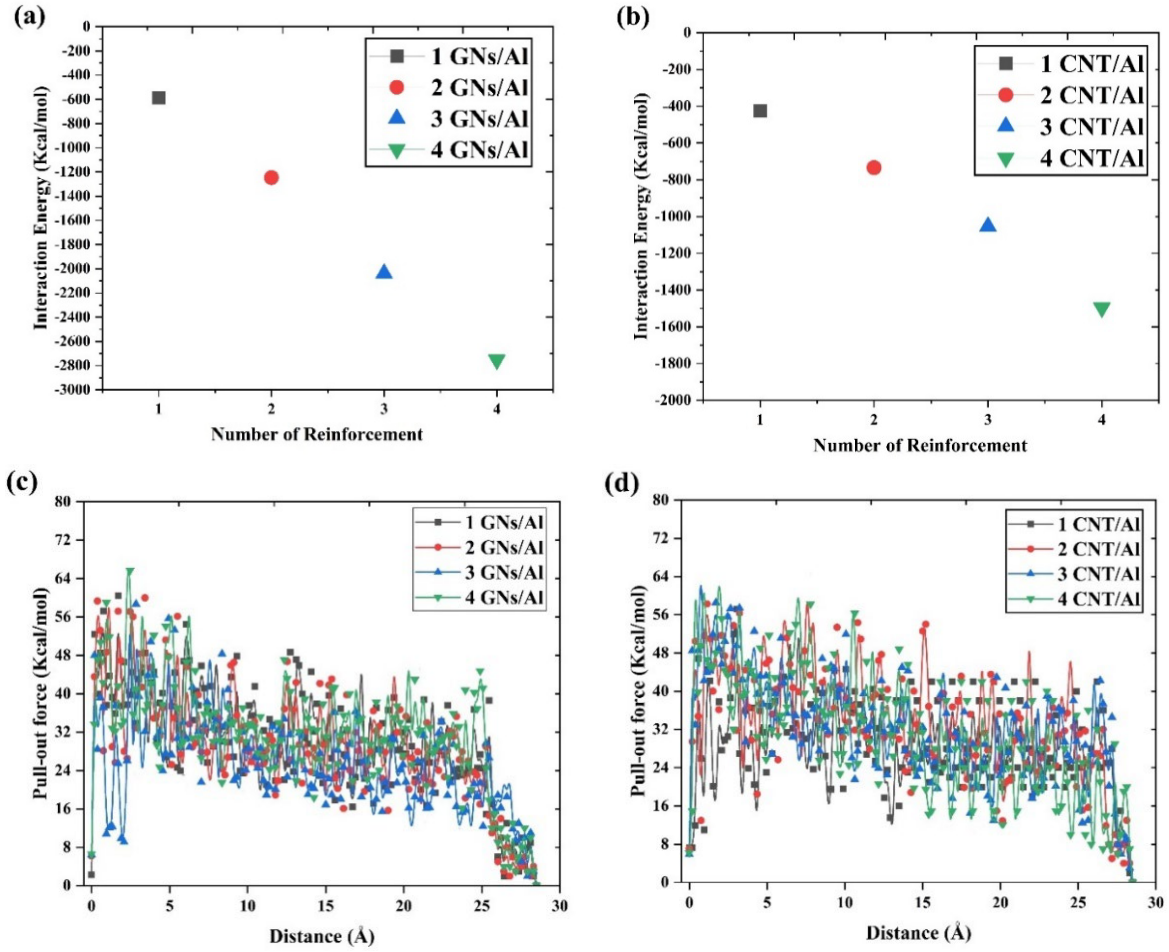

Figure 4. The amount of interaction energy (adhesion) and pullout force of aluminium nanocomposites reinforced with several graphene nanoplates and carbon nanotubes.

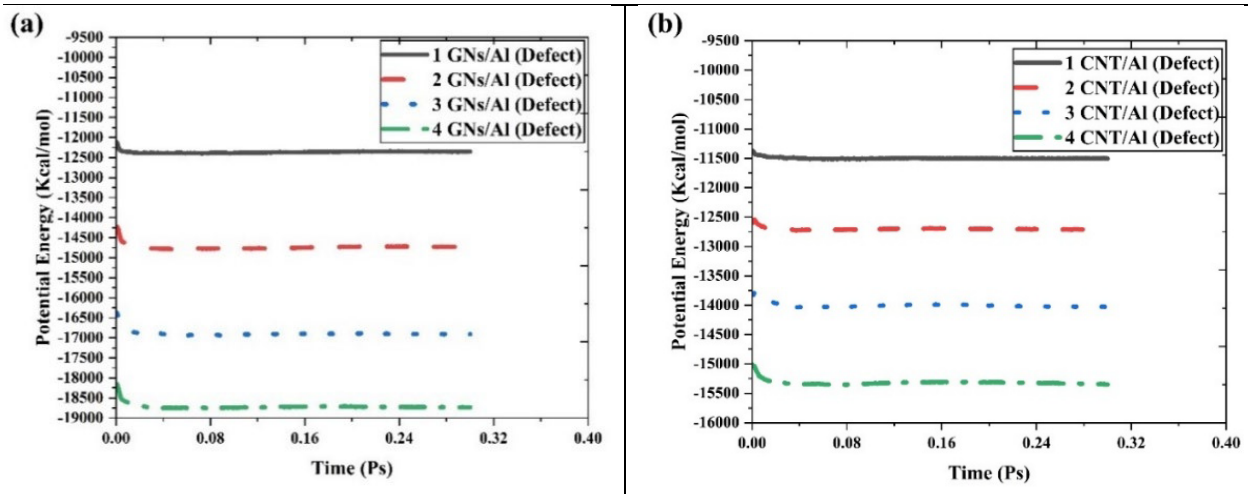

Figure 5. The potential energy of aluminium nanocomposites reinforced with several defective graphene nanoplates and carbon nanotubes.

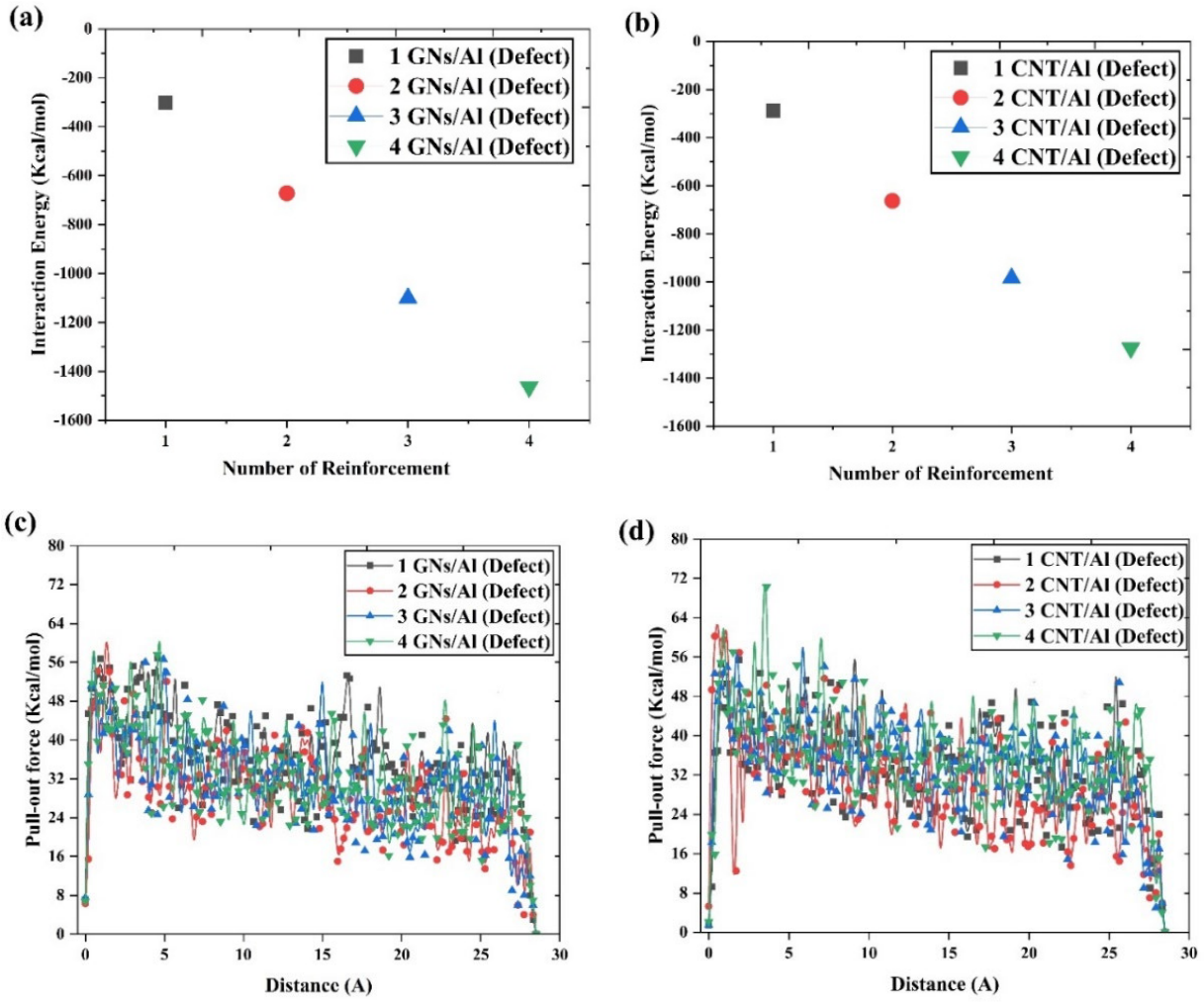

Figure 6. The interaction energy and pullout force of aluminium nanocomposites reinforced with several defective graphene nanoplates and carbon nanotubes.

(adhesion) between the carbon nanotubes and graphene nanoplates with the aluminium matrix increases.

The results obtained from the effect of increasing the number of reinforcements on the adhesion and interaction energy with the aluminium matrix are in good agreement with the results of Peng and Sun. [26] On the interfacial properties between graphene nano-reinforcers and copper matrix. In addition, by adding graphene nanosheets to the aluminium matrix, the amount of interaction energy (adhesion) increases. This result is in good agreement with the experimental results on copper matrix reinforcement with graphene nanosheets by Chu and Jia. [27].

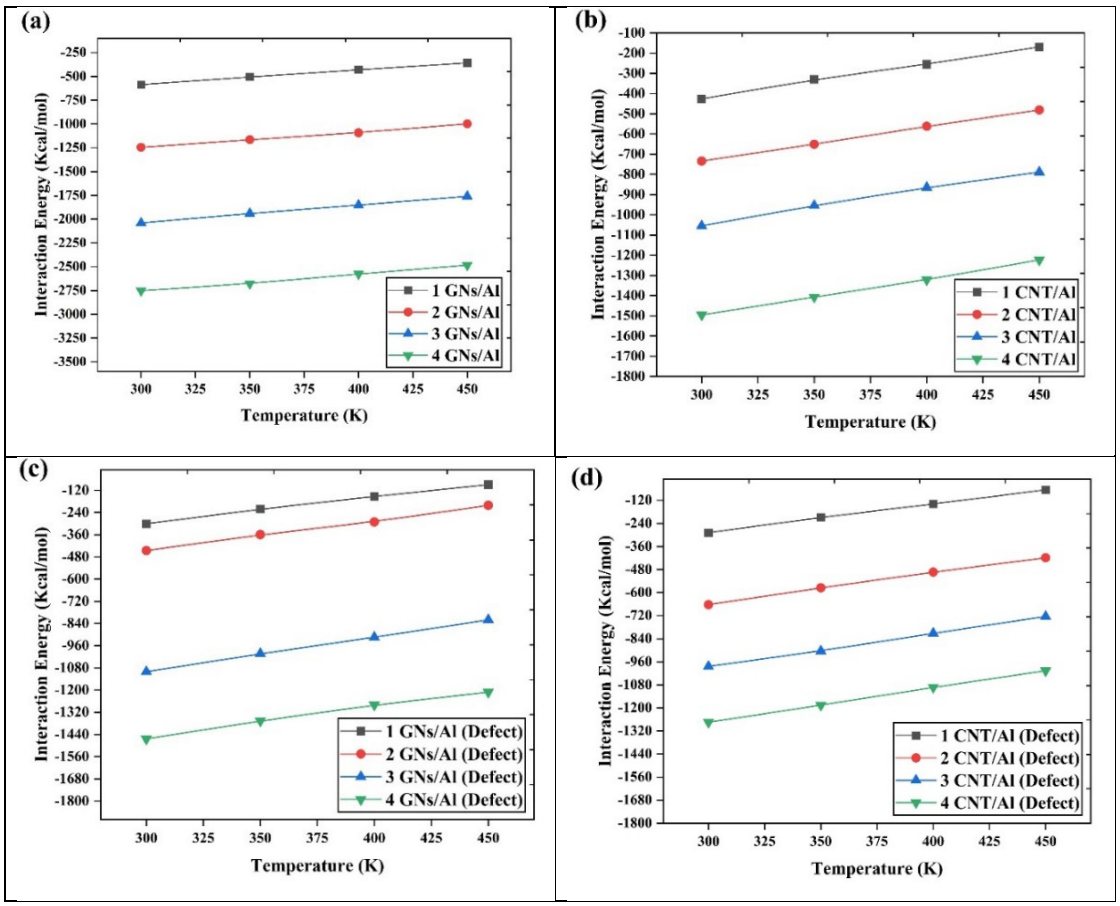

Figure 7. The interaction energy of aluminium nanocomposites reinforced with several graphene nanosheets and carbon nanotubes (with and without defects) under different temperatures.

3.2. The effect of defects in reinforcements on the interfacial properties of aluminium nanocomposites

Figure 5 shows the diagram and scale of the potential energy of aluminium nanocomposites reinforced with several defective graphene nanoplates and defective carbon nanotubes. According to diagrams a and b, increasing the number of reinforcements in the aluminium matrix, the amount of potential energy for defective graphene nanoplates and defective carbon nanotubes decreases from -12300 to -18750 Kcal/mol and -11100 to -15250 Kcal/mol, respectively.

In addition, Figure 6, parts a and b, shows the interaction energy of aluminium nanocomposites reinforced with several defective graphene nanoplates and defective carbon nanotubes.

According to Figure 6, parts a and b, by increasing the number of reinforcements from 1 to 4, the interaction energy for aluminium nanocomposites reinforced with graphene increases from -300 to -1500 Kcal/mol, and for aluminium nanocomposites reinforced with carbon nanotubes, it is from -270 to -1300 Kcal/mol. In addition, Figure 6 shows the pull-out force diagrams of aluminium nanocomposites reinforced with defective graphene nanoplates and defective carbon nanotubes. According to Figure 6, diagrams c and d, the highest amount of pull-out force is related to nanocomposites reinforced with 4 graphene layers, equal to 58 Kcal/mol, and 4 carbon nanotubes, equal to 67 Kcal/mol. Also, the lowest amount of pull-out force was 48 Kcal/mol for aluminium nanocomposites reinforced with one graphene layer and 47 Kcal/mol for one carbon nanotube.

Defects in nano-reinforcements were considered as a monovacancy defect (Figure 1). Also, these defects (Monovacancy defect) were added efficiently in the nanostructures as 1% for each graphene nanosheet or carbon nanotube. By adding the number of reinforcements (graphene nanosheets and carbon nanotubes) in nanocomposites, the percentage of defects also increases. The existence of defects in nano-reinforcement causes the failure of covalent bonds between carbon atoms in graphene nanosheets and carbon nanotubes. Therefore, the van der Waals and electrostatic forces between the aluminium matrix of the reinforcement are reduced. These results were also consistent with those of Li et al. [28] in the interfacial properties between defective reinforcements and epoxy matrix in composites.

3.3. Effect of temperature on aluminium nanocomposites reinforced with graphene nanoplates and carbon nanotubes

Figure 7 shows the interaction energy diagrams of aluminium nanocomposites reinforced with several graphene nanosheets and carbon nanotubes (with and without defects) formed under different temperatures.

According to Figure 7, diagrams a and b, with increasing temperature, the amount of interaction energy decreases between the aluminium matrix and graphene nanosheets

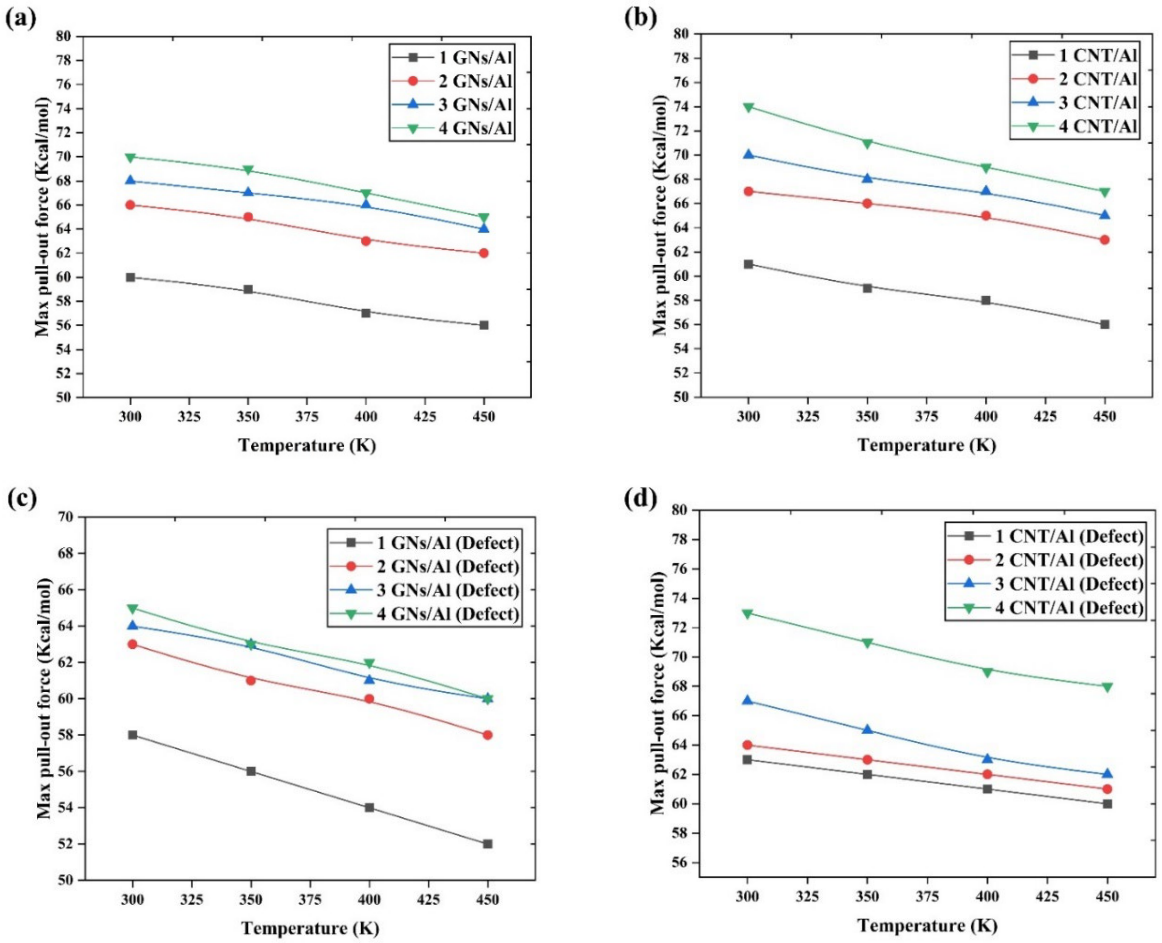

Figure 8. The maximum pull-out force diagrams of aluminium nanocomposites reinforced with several graphene nanoplates and carbon nanotubes (with and without defects).

as well as carbon nanotubes. Also, in Figure 7, diagrams c and d, with increasing temperature, the amount of interaction energy for aluminium nanocomposites reinforced with defective graphene nanoplates and defective carbon nanotubes decreases.

In addition, Figure 8 shows the maximum pull-out force diagrams of aluminium nanocomposites reinforced with several graphene nanoplates and carbon nanotubes (with and without defects). According to diagrams a, b, c, and d, by increasing temperature, the maximum pull-out force decreases in nanocomposites. According to Figure 8, the highest maximum pull-out force at 300 K is related to aluminium nanocomposites reinforced with 4 graphene nanoplates (70 kcal/mol), 4 defective graphene nanoplates (65 kcal/mol), 4 carbon nanotubes (74 kcal/mol), and 4 defective carbon nanotubes (72 kcal/mol).

As the temperature increases, the kinetic energy between the carbon atoms in the nano-reinforcements and the aluminium atoms in the matrix also increases. This causes the aluminium matrix to transition slightly from a solid to a more liquid (softer) state. As a result, the aluminium atoms become more delocalized, the van der Waals and electrostatic forces weaken. Therefore, it reduces adhesion (interaction energy) when separated from each other. This makes nanocomposites. The results of the molecular dynamics of this study were also consistent with the results of increasing the temperature of graphene-reinforced nanocomposites. [29, 30].

Conclusion

In this study, molecular dynamics simulation was used to investigate the interfacial properties between the aluminium matrix and graphene nanoplates, and carbon nanotubes (with and without defects). The results of this study show that by increasing the number of graphene nanosheets from 1 to 4, the amount of interaction energy and maximum pull-out force improved.

The highest interaction energy and maximum pull-out force are related to nanocomposites reinforced with 4 graphene nanoplates and 4 carbon nanotubes. In addition, the presence of defects in the structure of carbon nanotubes and graphene nanoplates reduces the interaction energy (adhesion) and the maximum pull-out force of aluminium nanocomposites. In addition, with the increase in temperature, the amount of interaction energy (adhesion) and maximum pull-out force between the aluminium matrix, graphene nanoplates, and carbon nanotubes decreased. The findings of this study offer a deeper insight into the interfacial properties (adhesion) between the reinforcements (graphene nanosheets and carbon nanotubes) and the aluminium matrix. Moreover, these results can assist in selecting the appropriate type and quantity of reinforcements for aluminium nanocomposites. This is because understanding the interfacial properties between the reinforcements and the aluminium matrix is closely linked to the mechanical properties of the nanocomposites.

Conflicts of interest

The authors declare that they have no conflict of interest.

References

1. Long R, Boettcher E, Crawford D. Current and future uses of aluminum in the automotive industry. JOM. 2017;69:2635-9. https://doi.org/10.1007/s11837-017-2554-9
2. Zhang A, Li Y. Thermal conductivity of aluminium alloys-A review. Materials (Basel). 2023;16:2972. https://doi.org/10.3390/ma16082972
3. Baiseitov D, Akhinzhanova A, Sassykova L, Avdonkina I, Tulepov M, Rassulova I. Development of a Marking Composition Based on Nanoaluminum and Iron Ore Concentrate for Mixed Explosives and Their Subsequent Identification. Int J Nanosci Nanotechnol. 2024;20:91-102.
4. Denisaev A, Shteinberg A, Berlin A. Initiation of a reaction in aluminum-Teflon multilayer thin-film samples by drop-hammer impact loading. Russ J Phys Chem B. 2008;2:491-7. https://doi.org/10.1134/S199079310803024X
5. Paik JK, Thayamballi AK, Kim GS. The strength characteristics of aluminum honeycomb sandwich panels. Thin Wall Struct. 1999;35:205-31. https://doi.org/10.1016/S0263-8231(99)00026-9
6. Rana R, Purohit R, Das S. Reviews on the influences of alloying elements on the microstructure and mechanical properties of aluminium alloys and aluminium alloy composites. Int J Sci Res Publ. 2012;2:1-7.
7. Novoselov KS, Geim AK, Morozov SV, Jiang D, Zhang Y, Dubonos SV, et al. Electric field effect in atomically thin carbon films. Science. 2004;306(5696):666-9. https://doi.org/10.1126/science.1102896
8. De Volder MF, Tawfick SH, Baughman RH, Hart AJ. Carbon nanotubes: present and future commercial applications. Science. 2013;339(6119):535-9. https://doi.org/10.1126/science.1222453
9. Geim AK, Novoselov KS. The rise of graphene. Nat Mater. 2007;6:183-91. https://doi.org/10.1038/nmat1849
10. Salehi A, Rash-Ahmadi S. Influence of oxygen functional groups on the crack growth behavior of graphene with edge and middle crack: A molecular dynamics study. Proc Inst Mech Eng N J Nanomater Nanoeng Nanosyst. 2024;23977914231217920.
11. Salehi A, Ghaderiazar N, Rash-Ahmadi S. Investigation of thermal conductivity and mechanical properties in multi-layer of graphene and graphene oxide: a molecular dynamics study. Mol Simul. 2024;50:954-68. https://doi.org/10.1080/08927022.2024.2369710
12. Kumar S. Graphene engendered 2-D structural morphology of aluminum atoms: Molecular dynamics simulation study. Mater Chem Phys. 2017;202:329-39. https://doi.org/10.1016/j.matchemphys.2017.09.043
13. Jiang W-G, Wu Y, Qin Q-H, Li D-S, Liu X-B, Fu M-F. A molecular dynamics based cohesive zone model for predicting interfacial properties between graphene coating and aluminium. Comput Mater Sci. 2018;151:117-23. https://doi.org/10.1016/j.commatsci.2018.05.008
14. Kumar S. Graphene Engendered aluminum crystal growth and mechanical properties of its composite: An atomistic investigation. Mater Chem Phys. 2018;208:41-8. https://doi.org/10.1016/j.matchemphys.2018.01.013
15. Kumar S, Pattanayek SK, Das SK. Reactivity-controlled aggregation of graphene nanoflakes in aluminum matrix: atomistic molecular dynamics simulation. J Phys Chem C. 2019;123:18017-27. https://doi.org/10.1021/acs.jpcc.9b03101
16. Li J, Zhang X, Geng L. Effect of heat treatment on interfacial bonding and strengthening efficiency of graphene in GNP/Al composites. Compos Part A Appl Sci Manuf. 2019;121:487-98. https://doi.org/10.1016/j.compositesa.2019.04.010
17. Li R, Pan Z, Zeng Q, Xiaoli Y. Influence of the interface of carbon nanotube-reinforced aluminum matrix composites on the mechanical properties-a review. Arch Foundry Eng. 2022;22:23-36. https://doi.org/10.24425/afe.2022.140213
18. Guarda C, Faria B, Silvestre N, Lopes JNC. Influence of matrix recrystallization and nanofiller porosity on the interfacial properties of holey graphene-aluminium nanocomposites. Compos Struct. 2023;312:116856. https://doi.org/10.1016/j.compstruct.2023.116856
19. Rafiee J, Wang Z, Song H, Yu Z-Z, Koratkar N, Reif J. Enhanced mechanical properties of nanocomposites at low graphene content. ACS Nano. 2009;3:3884-90. https://doi.org/10.1021/nn9010472
20. Zhang X, Chen H, Qiao D, Yang M. Effects of structure defects on thermal transport at the graphene-water interface. Adv Mater Interfaces. 2023;10:2202518. https://doi.org/10.1002/admi.202202518
21. Tersoff J. New empirical approach for the structure and energy of covalent systems. Phys Rev B. 1988;37:6991. https://doi.org/10.1103/PhysRevB.37.6991
22. Daw MS, Baskes MI. Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. Phys Rev B. 1984;29:6443. https://doi.org/10.1103/PhysRevB.29.6443
23. Plimpton S. Fast parallel algorithms for short-range molecular dynamics. J Comput Phys. 1995;117:1-19. https://doi.org/10.1006/jcph.1995.1039
24. Salehi A, Rash-Ahmadi S. Effect of adsorption, hardener, and temperature on mechanical properties of epoxy nanocomposites with functionalized graphene: A molecular dynamics study. J Mol Graph Model. 2022;117:108311. https://doi.org/10.1016/j.jmgm.2022.108311
25. Sun S, Chen S, Weng X, Shan F, Hu S. Effect of carbon nanotube addition on the interfacial adhesion between graphene and epoxy: A molecular dynamics simulation. Polymers (Basel). 2019;11:121. https://doi.org/10.3390/polym11010121
26. Peng W, Sun K. Effects of Cu/graphene interface on the mechanical properties of multilayer Cu/graphene composites. Mater Sci Eng A Struct Mater. 2020;141:103270. https://doi.org/10.1016/j.mechmat.2019.103270
27. Chu K, Jia C. Enhanced strength in bulk graphene-copper composites. Phys Status Solidi A Appl Mater Sci. 2014;211:184-90. https://doi.org/10.1002/pssa.201330051
28. Li M, Zhou H, Zhang Y, Liao Y, Zhou H. The effect of defects on the interfacial mechanical properties of graphene/epoxy composites. RSC Adv. 2017;7:46101-8. https://doi.org/10.1039/C7RA08243F
29. Lu P, Chen H, Zhang J, Xiao G, Yi M, Chen Z. Effects of graphene pull-out on the interfacial mechanical properties of alumina/graphene nanocomposite ceramic tool materials: Molecular dynamics analysis and material preparation. Int J Appl Ceram Technol. 2024;21:451-64. https://doi.org/10.1111/ijac.14525
30. Salehi A, Rash-Ahmadi S. Effect of temperature and oxygen functional groups on interaction between epoxy resins and graphene surface. Proc Inst Mech Eng C J Mech Eng Sci. 2023;237:941-51. https://doi.org/10.1177/09544062221126626