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# Simulation of graphene adding effect on theimprovementof the mechanicalproperties of aluminum-graphene nanocomposites

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**Abstract:** Aluminum, a light metal with high strength to weight ratio, low price and low density can have a wide application as a matrix in the metal matrix composites, but its usage is limited because of having low yield strength. Aluminum matrix composites strengthened by graphene, can be an excellent research subject in order to improve mechanical properties of Al alloys. Due to discontinuity in nanoscale, continuum mechanics theories can't be used for investigating such systems. The best alternative for studying such systems is application of the molecular dynamics method which is based on classical mechanics and reliable software collections have been developed for it. In this research, molecular dynamics (MD) simulation of aluminum-graphene nanocomposite (Al-Gr) is done. The mechanical properties of aluminum-graphene nanocomposite and the most significant factors were investigated by applying uniaxial load and stretching on its ends. The interactions between aluminum atoms were modeled using embedded atom potential method (EAM) and AIREBO potential was used for the interactions of Carbon atoms. These two potentials are accompanied by the Lennard-Jones (LJ) potential. Computational results show that modulus of elasticity and tensile strength of aluminum-graphene composites are getting increased by increasing the weight percent of graphene to aluminum, decreasing the temperature, increasing load speed and decreasing the size of defects. These observations are in agreement with the observed phenomena in the macroscale experiments. Results from the molecular dynamics simulations are also compared with analytical results obtained from semi-empirical Halphin-Tsai (H-T) model and the Rule of Mixtures (ROM).

**Keywords:** Molecular dynamics (MD); Aluminum; graphene; Nanocomposite; Mechanical properties