Abstract

iMedPub Journals
www.imedpub.com

Nano Research & Applications
ISSN 2471-9838

2021
Vol.7 No: S2

MD-based design of Sic/graphene Nano composites towards better mechanical performance

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Abstract

In this study, molecular dynamics (MD) simulation has been implemented to explore the main parameters affecting the reinforcing role of graphene in ceramic-based composites. Due to the importance of silicon carbide in industrial applications, this ceramic has been considered as the matrix material. Uniaxial tensile test is employed to analyze the mechanical behavior of this type of nanocomposites. Accordingly, the stress-strain curve can be achieved for each sample from which different mechanical properties including Young's modulus, ultimate tensile strength, failure strain, and fracture toughness can be achieved. This is followed by investigation of the reinforcing role of graphene at different temperatures. In the present work, single layer graphene sheet (SLGS) and its double layer counterpart has been utilized as the reinforcing agent at two different volume fractions (VFs) of 3% and 5%. Results show that increasing the VF of SLGS up to 5%, causes an enhancement in the Young modulus by 31.7%. Additionally, it is found that increasing the number of graphene layers has a detrimental effect on the mechanical behavior of mentioned nanocomposite samples. This is attributed to the interlayer sliding occurred between graphene layers due to the weak van der Waals interactions operating between them. Finally, the dominant mechanism of the fracture toughness of these nanocomposites is systematically studied through various case studies.

Biography

Mohsen Barfmal studied his Master of Science - M.Sc, Materials Engineering from K. N. Toosi University of Technology,Iran.