عنوان مقاله:

Machine Learning Insights into the Influence of Carbon Nanotube Dimensions on Nanocomposite Properties : A Comprehensive Exploration

محل انتشار:

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نویسندگان:

Atefeh Zarei – School of Systems and Enterprises, Stevens Institute of Technology, Hoboken, NJ, USA

Ashkan Farazin – Department of Mechanical Engineering, Stevens Institute of Technology, Castle Point on Hudson, Hoboken, NJ, ۰۷۰۳۰, USA

خلاصه مقاله:

Multiscale modeling (MM) has broadened its scope to encompass the calculation of mechanical properties, with a particular focus on investigating how the dimensions of single-walled carbon nanotubes (SWCNTs), specifically their diameters, affect the mechanical properties (Longitudinal and Transverse Young's modulus) of simulated nanocomposites through Molecular Dynamics (MD) simulations. The MD method was employed to construct nanocomposite models comprising five different SWCNTs chiralities : (۵, ۰), (۱۰, ۰), (۱۵, ۰), (۲۰, ۰), and (۲۵, ۰), serving as reinforcements within a common Polymethyl methacrylate (PMMA) matrix. The findings indicate a correlation between the SWCNT diameter increase and enhancements in mechanical and physical properties. Notably, as the diameter of SWCNTs increases, the density, Longitudinal Young's modulus, Transvers Young's Shear modulus, Poisson's ratio, and Bulk modulus of the simulated nanocomposite transition from (۵, ۰) to (۲۵, ۰) by approximately ۱.۵۴, ۳, ۲, ۱.۴۳, ۱.۱۱, and ۱.۷۵ times, respectively. To corroborate these results, stiffness matrices were derived using Materials Studio soft ware.

کلمات کلیدی:

Molecular dynamics simulation, Mechanical properties, Polymethyl methacrylate, single walled carbon nanotubes