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Computational Design of Epoxy/ Boron Carbide Nanocomposites for Radiation Shielding Applications. KARTEEK BEJAGAM, Virginia Tech , NASIM GALEHDARI, INGRID ESPINOSA, Ph.D Student, SANKET A. DESHMUKH, Assistant professor, AJIT D. KELKAR, Professor — An individual working in industries that include nuclear power plants, healthcare industry, and aerospace are knowingly or unknowingly exposed to radiations of different energies. Exposure to high-energy radiations such as α/β particle emissions or gamma ray electromagnetic radiations enhances the health risks that can lead to carcinogenesis, cardiac problems, cataracts, and other acute radiation syndromes. The best possible solution to protect one from the exposure to radiations is shielding. In the present study, we have developed a new algorithm to generate a range of different structures of Diglycidyl Ether of Bisphenol F (EPON 862) and curing agent Diethylene Toluene Diamine (DETDA) resins with varying degrees of crosslinking. 3, 5, and 10 weight percent boron carbide was employed as filling materials to study its influence on the thermal and mechanical properties of composite. We further conduct the reactive molecular dynamics (RMD) simulations to investigate the effect of radiation exposure on the structural, physical, and mechanical properties of these Epoxy/Boron Carbide nanocomposites. Where possible the simulation results were compared with the experimental data.

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