Examination of the mechanical properties of porous carbon matrix by considering the Nanovoids: A computational study using molecular dynamics simulation

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Abstract

This study explored the effect of nanovoid size on the mechanical properties of polymer-carbon matrices through detailed molecular dynamics simulations. The investigation focused on spherical nanovoids with radii of 5, 7, 10, 12, and 15 Å, evaluating their effects on critical mechanical properties, such as Young's modulus and ultimate strength. The Tersoff potential was employed to accurately model the atomic and mechanical behavior of the polymer-carbon matrix, considering the presence of these nanovoids. The simulation results indicate that the potential energy and total energy stabilized at −132,279.23 eV and − 131,522.4 eV, respectively, confirming the physical stability of simulated samples. On the other hand, the findings reveal that for a nanovoid radius of 5 Å, the ultimate strength and Young's modulus were 36.41 GPa and 424.93 GPa, respectively. As the radius of nanovoids increased from 5 Å to 15 Å, both ultimate strength and Young's modulus exhibited a decreasing trend, with values dropping from 36.41 GPa and 424.93 GPa to 31.18 GPa and 364.39 GPa, respectively. Moreover, larger nanovoids contributed to increased flexibility and a higher critical strain in the polymer-carbon matrix. This systematic analysis of nanovoid size effects provided a new perspective on void engineering within composites. By enhancing the theoretical understanding of how void dimensions affected material properties, the study offered significant insights for optimizing the mechanical performance of advanced materials and advancing the field of structural engineering.