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STRENGTH AND FAILURE MECHANISMS OF CNT-REINFORCED COPPER NANOCOMPOSITE

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Abstract

This paper presents a study on the mechanical behaviour of copper (Cu) nanocomposites reinforced with carbon nanotubes (CNTs) using Molecular Dynamics (MD). Tensile and compressive loadings are applied to two limit boundary conditions of CNT: (i) case A – loading applied to the Cu matrix (the embedded CNT is not loaded) and (ii) case B – loading applied to both Cu matrix and embedded CNT. The reference case (Cu matrix without CNT) is also considered. Curves of energy and stress vs. strain are presented and mechanical properties (Young's modulus, yield stresses and strains) are calculated. In the first case, the CNT has an overall detrimental effect to the CNT-Cu nanocomposite, reducing yield strains and stresses, while showing residual effect to the Young's modulus. In the second case, the Young's modulus and strengths (tensile and compressive) increase reasonably while the yield strains decrease fairly. This study shows that the CNT might increase the stiffness and strength of the nanocomposite, but also decrease its ductility. Additionally, this work also reports atomic stress distributions, dislocation patterns and crystalline structures of the loaded CNT-Cu nanocomposite, which explain not only the failure mechanisms but also the differences between compressive and tensile behaviours.

Keywords: Nanocomposites, Carbon nanotubes (CNT), Copper, Mechanical properties, Molecular dynamics (MD), dislocations, failure mechanisms