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Nanoporous Gold Reinforced with Carbon Based Nanomaterials: A Molecular Dynamics Study

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Abstract

Considering the fact that carbon based nanostructures (CBNs) and nanoporous (np) metals are very promising for future applications, the main motivation of this study is to improve the mechanical characteristics of np metals by employing CBNs including graphene nanoribbons (GNRs), fullerenes and CNTs within the cellular voids by presenting a new metal-carbon nanocomposite material. For this purpose, a Voronoi-based atomistic modeling technique is used to obtain numerical models of the proposed hybrid structures and their mechanical properties under tensile and compressive loading conditions are investigated by classical molecular dynamics. Instead of reinforcing with discrete units, a heat welding procedure is applied to generate a covalently bonded network of carbon based structures. Results clearly indicate that the utilization of carbon based nanostructures enhances both tensile and compressive response of np metals significantly while a minor microstructural change is observed within the crystal structure. The major effect is observed especially on the yield and post-yield behavior of np structures, while the elastic modulus is not affected remarkably. The main reason for the enhancement is greatly attributed to the covalent bonding generated