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Nanoporous Metals Reinforced with Fullerenes

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Abstract : Nanoporous (np) metals have attracted considerable attention owing to their cellular morphological features at atomistic scale which yield ultra-high specific surface area awarding a great potential to be employed in diverse applications such as catalytic, electrocatalytic, sensing, mechanical and optical. As one of the carbon based nanostructures, fullerenes are also another type of outstanding nanomaterials that have been extensively investigated due to their remarkable chemical, mechanical and optical properties. In this study, the idea of improving the mechanical behavior of nanoporous metals by inclusion of the fullerenes, which offers a new metal-carbon nanocomposite material, is examined and discussed. With this motivation, tensile mechanical behavior of nanoporous metals reinforced with carbon fullerenes is investigated by classical molecular dynamics (MD) simulations. Atomistic models of the nanoporous metals with ultrathin ligaments are obtained through a stochastic process simply based on the intersection of spherical volumes which has been used previously in literature. According to this technique, the atoms within the ensemble of intersecting spherical volumes is removed from the pristine solid block of the selected metal, which results in porous structures with spherical cells. Following this, fullerene units are added into the cellular voids to obtain final atomistic configurations for the numerical tensile tests. Several numerical specimens are prepared with different number of fullerenes per cell and with varied fullerene sizes. LAMMPS code was used to perform classical MD simulations to conduct uniaxial tension experiments on np models filled by fullerenes. The interactions between the metal atoms are modeled by using embedded atomic method (EAM) while adaptive intermolecular reactive empirical bond order (AIREBO) potential is employed for the interaction of carbon atoms. Furthermore, atomic interactions between the metal and carbon atoms are represented by Lennard-Jones potential with appropriate parameters. In conclusion, the ultimate goal of the study is to present the effects of fullerenes embedded into the cellular structure of np metals on the tensile response of the porous metals. The results are believed to be informative and instructive for the experimentalists to synthesize hybrid nanoporous materials with improved properties and multifunctional characteristics.

Keywords : fullerene, intersecting spheres, molecular dynamic, nanoporous metals
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