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Ab Initio Approach to Generate a Binary Bulk Metallic Glass Foam

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Abstract : Both porous materials and bulk metallic glasses have been studied due to their potential applications and their exceptional physical and chemical properties. However, each material presents certain drawbacks which have been thought to be overcome by generating bulk metallic glass foams (BMGF). Although some experimental reports have been performed on multicomponent BMGF, still no ab initio works have been published, as far as we know. We present an approach based on the expanding lattice (EL) method to generate binary amorphous nanoporous Cu64Zr36. Starting from two different configurations: a 108-atom crystalline cubic supercell (cCu64Zr36) and a 108-atom amorphous supercell (aCu64Zr36), both with an initial density of 8.06 g/cm3, we applied EL method to halve the density and to get 50% of porosity. After the lattice expansion the supercells were subject to ab initio molecular dynamics for 500 steps at constant room temperature. Then, the samples were geometry-optimized and characterized with the pair and radial distribution functions, bond-angle distributions and a coordination number analysis. We found that pores appeared along specific spatial directions different from one to another and that they differed in size and form as well, which we think is related to the initial structure. Due to the lack of experimental counterparts our results should be considered predictive and further studies are needed in order to handle a larger number of atoms and its implication on pore topology.

Keywords : ab initio molecular dynamics, bulk mettalic glass, porous alloy
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