World Academy of Science, Engineering and Technology
International Journal of Mechanical and Materials Engineering
Vol:10, No:08, 2016

Effects of Nano-Coating on the Mechanical Behavior of Nanoporous Metals

Authors : Yunus Onur Yildiz, Mesut Kirca

Abstract : In this study, mechanical properties of a nanoporous metal coated with a different metallic material are studied through a new atomistic modelling technique and molecular dynamics (MD) simulations. This new atomistic modelling technique is based on the Voronoi tessellation method for the purpose of geometric representation of the ligaments. With the proposed technique, atomistic models of nanoporous metals which have randomly oriented ligaments with non-uniform mass distribution along the ligament axis can be generated by enabling researchers to control both ligament length and diameter. Furthermore, by the utilization of this technique, atomistic models of coated nanoporous materials can be numerically obtained for further mechanical or thermal characterization. In general, this study consists of two stages. At the first stage, we use algorithms developed for generating atomic coordinates of the coated nanoporous material. In this regard, coordinates of randomly distributed points are determined in a controlled way to be employed in the establishment of the Voronoi tessellation, which results in randomly oriented and intersected line segments. Then, line segment representation of the Voronoi tessellation is transformed to atomic structure by a special process. This special process includes generation of non-uniform volumetric core region in which atoms can be generated based on a specific crystal structure. As an extension, this technique can be used for coating of nanoporous structures by creating another volumetric region encapsulating the core region in which atoms for the coating material are generated. The ultimate goal of the study at this stage is to generate atomic coordinates that can be employed in the MD simulations of randomly organized coated nanoporous structures. At the second stage of the study, mechanical behavior of the coated nanoporous models is investigated by examining deformation mechanisms through MD simulations. In this way, the effect of coating on the mechanical behavior of the selected material couple is investigated.

Keywords : atomistic modelling, molecular dynamic, nanoporous metals, voronoi tessellation
Conference Title : ICTAMM 2016 : International Conference on Theoretical and Applied Multiscale Mechanics
Conference Location : Amsterdam, Netherlands
Conference Dates : August 04-05, 2016