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Influence of voids distribution on the deformation behavior of nanocrystalline palladium

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Abstract

Uniaxial deformation of three-dimensional nanocrystalline palladium containing porosity in the form of voids was investigated by means of molecular dynamics method. Simulations were performed at temperature of 300 K and at a constant strain rate of $10^8 \, \mathrm{s}^{-1}$. Two cases of voids distribution were considered: random and at triple or quadrupole junctions. It has been revealed that both the voids distribution and subsequent annealing at elevated temperature influence the deformation behavior of nanocrystalline palladium. In particular, the presence of voids at triple junctions results in a reduction of the Young's modulus and more pronounced softening effect during plastic deformation. The subsequent annealing evokes shrinkage of voids and strengthening effect. Contribution of grain boundary accommodation processes into both elastic and plastic deformation of nanocrystalline materials is discussed.

Keywords: Nanocrystalline Materials; Mechanical Properties; Voids; Molecular Dynamics Simulation

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