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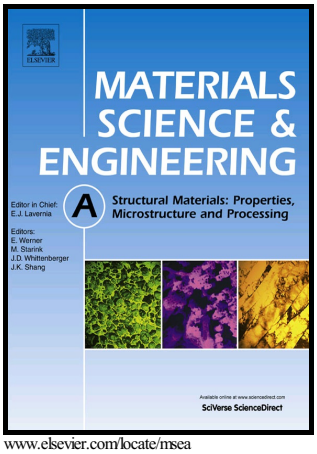

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ACCEPTED MANUSCRIPT

INFLUENCE OF INTERNAL STRESSES ON DEFORMATION BEHAVIOR OF NANOCRYSTALLINE PALLADIUM

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Abstract

Molecular dynamics simulations of internal stress influence on deformation behavior of three-dimensional nanocrystalline palladium structure were performed at room temperature and at a constant strain rate. In order to achieve a different level of internal stresses, a predeformed sample was held at a fixed size along the direction of compressive straining during 50 and 500 ps. Thereafter these two samples with different states of non-equilibrium structure were further deformed along the same direction. It turned out that internal stresses influence the deformation behavior of nanocrystalline palladium, in particular, an increase of the stress relaxation time results in a growth of the ultimate strength. Relaxation of non-equilibrium structure and transition to a more equilibrium state in terms of reduction of both the internal stresses and free volume are analyzed.

Keywords: nanocrystalline materials; uniaxial compressive straining; grain boundaries; stress relaxation; molecular dynamics simulation.

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