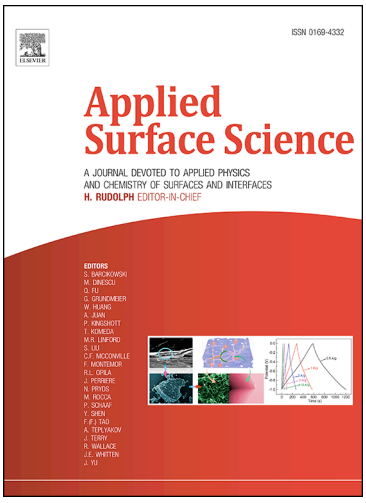

Full Length Article

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Abstract

The properties and performance of TiN thin films are closely related to the concentration and mobility of lattice defects in the thin film structures of TiN. This makes a local atomic scale study of TiN thin films an ever-growing demand. Emission ^{57}Fe Mössbauer spectroscopy (eMS) is a powerful tool in this regard, which we apply here to study an ultrathin TiN film epitaxially grown on MgO (100). With the help of theoretical calculations, our results show that most implanted Fe ions adopt a 2^+ valence state and locate at the Ti sublattice in the bulk-like single crystalline grains, with the rest Fe residing at the grain boundaries as interstitials. A small percentage of nitrogen point defects (vacancy V_N and interstitial N_I) are observed in the bulk-like crystalline grains. A temperature-dependent, interstitial N_I mediated site-exchange between N_I and V_N inside the crystal grain are deduced via a N_2 dimmer like diffusion of N_I through the crystal grains in the temperature range of 540 - 620 K. This is interesting in the perspective of exploring the catalytic property of TiN nanostructures. The titanium vacancy (V_{Ti}) is only detected at the grain boundaries. Annealing up to 813 K, both the V_N and N_I are annihilated in the crystalline grains and the V_{Ti} is fully recovered with healing of the grain boundaries. However, no evidence of ferromagnetism due to dilute implantation of ^{57}Mn/^{57}Fe and or structural defects in the film is obtained.