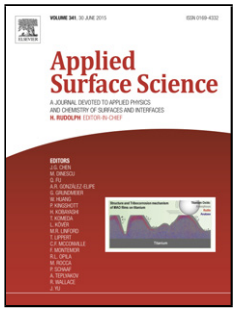

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Numerical investigation of sputtering power effect on nano-tribological properties of tantalum-nitride film using molecular dynamics simulation

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highlights

- Surface roughness variation reaches to a minimum with increasing power density and then starts to increase.
- Increasing deposition rate leads to harder surface diffusion and less kinetic energy.
- Increasing the incident energy increases the kinetic energy and hence reduces surface diffusion.
- Harder surface diffusion and less kinetic energy of atoms cause the surface to roughen.

Abstract

In the present work, surface profile of tantalum-nitride films, deposited with different sputtering power is analyzed using atomic force microscopy (AFM) in order to find out the effect of sputtering power density on the surface properties. In this regard, micron size tantalum nitride films were deposited using reactive magnetron sputtering system with sputtering power density of 1.5 to 3 W/cm^2 in argon environment mixed with nitrogen. The process was then simulated numerically using molecular dynamics simulation (MD) and Morse interatomic potential in order to study the mechanism of surface roughness variation with sputtering power. According to experimental results, with increasing the sputtering power density from 1.5 to 3, the surface roughness decreased at first followed by an increase. The reason of this behavior was investigated using MD simulation. In this regard, the effect of sputtering power was attributed into two different phenomena: i) the deposition rate and ii) the incident-atom energy. Simulation was performed at different deposition rates from 33 to 666 atoms/ps and different sputtered atom energies from .31 to 7.67 eV. It is found that increasing the incident-atom energy causes the atoms to move along the surface and reduces