Molecular dynamics study of sliding mechanisms of Ni, amorphous Ni-P and nanocrystalline Ni films

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ABSTRACT

Pure metal coatings are highly appreciated in many technical applications because of relative simple manufacturing technologies offering the opportunity to adjust film properties according to customers' needs by controlling processing parameters. Compared to copper and tin coatings nickel is a hard coating which often is used to increase the load carrying capacity of a substrate and thus improve its wear resistance [1]. Frequently, the improvement of hardness and wear resistance could be attributed to a reduction of grain size of electro-plated nickel coatings [2]. Whereas the effect of decreasing grain size on hardness and wear resistance is described by the Hall-Petch relationship, the effect of grain size on the coefficient of friction (COF) is not so well understood. It is plausible that amorphous grain boundary layers will also exert an impact on the tribological behavior, especially on the COF. The idea was to study the sliding behavior of amorphous nickel films supported by nickel crystals on both sides.

In the paper molecular dynamics modeling is used to investigate the sliding feature of different nano-scale specimens: single-crystal nickel evolving from amorphous pure Ni during shear deformation, Ni-P amorphous layer and nanocrystalline nickel. Special attentions are paid to the value of resistance stresses and plastic deformation mechanisms manifested during sliding simulations. The study is performed for considered systems at a temperature of about 300 K with narrow acceptable range of temperature fluctuation. It was found that Ni-P amorphous structure is characterized by lowest resistance stresses and smooth sliding provided by the bond-switching mechanism between pairs of atoms due to shear loading. Similar low resistance stress was also observed for an amorphous pure Ni layer, but only at an early stage of sliding before crystallization occurred. The highest shear resistance was confirmed for single-crystal nickel caused by classical deformation mechanisms like stacking fault formation and dislocation movement. Sliding simulations of a nanocrystalline specimen show both, crystal defect driven deformation in the bulk and sliding along quasi-amorphous grain boundaries. In that case the resistance force was between amorphous layer sliding and single crystal sliding, but closer to amorphous layer sliding.

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