

FIRST-PRINCIPLES CALCULATIONS AND INSIGHT OF MICROSTRUCTURAL EFFECTS ON MECHANICAL PROPERTIES IN THE HETEROSTRUCTURED (CrN/ZrN)/(Cr/Zr) NANOCOMPOSITE COATINGS

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Coatings with desirable properties of adhesion, strength and high wear performance can be achieved by depositing multilayered structures of Me/MeN architecture. Recent investigations have shown that the combination of hard but brittle metal nitride layers with tough but relatively soft metallic layers in multilayered “sandwich” improves the performance of the composite material for many reasons [1]. Herein, a sandwich (CrN/ZrN)/(Cr/Zr) nanocomposite coatings were synthesized by the vacuum-arc evaporation of the cathodes (Arc-PVD) in nitrogen atmosphere ($P_{N(CrN/ZrN)} = 0.53$ Pa, $P_{N(Cr/Zr)} = 0.003$ Pa). The highest value of hardness up to 29 GPa had been registered for the coatings of the series with the bilayers thickness relation of CrN/ZrN(1069 nm)/Cr/Zr(110 nm). The increase in hardness for (CrN/ZrN)/(Cr/Zr) coatings is mainly attributed to the high volume of boundary interfaces, the high number of interlayer interfaces and lattice parameter mismatch. The last is affect the total number of interfacial dislocations, hence, increases the required force to cause the deformation. Additionally, the thinness of the metallic layers also results in fewer dislocation formations and, hence, less accumulation of dislocations near the interfaces.

References

1. Abadias, G.; Michel, A.; Tromas, C.; Jaouen, C.; Dub,S. N. Stress, interfacial effects and mechanical properties of nanoscale multilayered coatings. *Surf. Coat. Technol.* 2007, 202, 844–853.