High temperature (up to 1200 °C) thermal mechanical stability of Si and Ni doped CrN framework coatings

ABSTRACT

High temperature thermal-mechanical stability of tribological thin coatings is extremely important to a large number of applications in modern industries. DC magnetron sputtering of single metallic element (Cr, Si) and alloy (Ni:Cr) targets formed transition metal nitrides film coatings, CrSiN and CrNiN onto M2 steel. High temperature in-situ synchrotron X-ray diffraction, in the range 25 °C-700 °C, obtained experimental data for a range of structural and mechanical properties. Furthermore, experimental room temperature Nanoindentation measurements, made before and after the in-situ heating cycle, provided corresponding hardness and shear modulus results. The structural results identified microstructure and phase transformation changes, while the mechanical results identified microstrain, hardness, elastic modulus and deformation resistance properties of the coatings. Density functional theory (DFT) and quasi-harmonic approximation (QHA) modelled the high temperature thermal and mechanical properties such as: Young's modulus, shear modulus and thermal expansion coefficients (populated up to 1200 °C). Estimates of hardness are made by correlating the bulk phase hardness and shear modulus, of the CrN and Ni phases, as a function of temperature. Results indicate that Si doping enhances the hardness of the CrN framework, increasing from 29 to 36 GPa and improves the coatings elastic modulus, and resistance to deformation. However, the addition of Ni reduced these properties. Furthermore, formation of (Cr,Si)N and Ni(Cr) solid solutions is inferred from DFT, Rietveld and lattice constant analysis.