Elastoplastic and microstructural properties of interfaces in metal-nitride multinanolayered coating using continuum mechanics and ab-initio methods

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Multilayer coatings have been widely used in industry since the late 1980s as protective coatings, particularly for cutting tools (PalDey and Deevi, 2003). One solution consists of depositing metal/nitride multilayered coatings to take advantage of the complementary properties of the nitride, the metal and the interfaces to enhance fracture toughness while maintaining very high hardness. Both hardness and fracture toughness of these coatings strongly depend on the stacking period: for some shorts periods, these mechanical properties are better (Pac et al., 2017). This phenomenon is controlled by the nature of the interface formed between layers. However, for nanometric period, the interfaces are too thin to be directly characterised mechanically or chemically. This work focuses on $Ti_{0.54}Al_{0.46}N$/ $Ti_{0.67}Al_{0.33}$ multilayer coatings (respectively labelled TiAlN and TiAl) deposited by Reactive Gas Pulsing Process (RGPP). Two approaches have been envisaged to characterise them. The first one is the quantification of each chemical species using a homogeneous finite element model. Transmission Electron Microscopy and Electron Energy Loss spectroscopy analysis reveal that nitrogen is often detected in TiAl closed to the interface, thus unbalancing the volume fraction of each component. Quantifying each chemical species using a homogenisation method therefore appears to be an essential tool. A finite element model of TiAl/TiAlN nano-multilayered coatings reproducing the mechanical behaviour during nanoindentation tests was developed. It uses an equivalent homogenised monolithic coating with an elastic-plastic behaviour based on a rule of mixture of both TiAl and TiAlN monolithic properties. The plastic behaviour was identified using a Finite Element Model Updating (FEMU) method from dual indentation technique. Only the volume fraction of TiAlN, is required to define an equivalent and homogenized multilayered coating and to reproduce both the experimental indentation curves and the hardness. It is observed that the value of the volume fraction of TiAlN is superior to the theoretical value, and increases as the period decreases, highlighting an imbalance in the proportion of each material. Then, a determination of the mechanical properties of the interface via ab-initio and molecular dynamics method to assess to the mechanical properties of the layer. Ab-initio methods (Density Functional Theory) simulations were used to determine a TiAl and a TiAlN structure with optimized hardness. Two TiAl/TiAlN interfaces were modelled, one with a TiAlN cubic growth direction of [111], the other with a cubic growth direction of [200] in accordance with X-ray

diffraction experimental observations. Since TiAl and TiAlN are not naturally congruent, molecular dynamics calculations were used to relax the interfaces and accommodate structural mismatches. Results show that the TiAl/TiAlN interfaces exhibit higher Vickers hardness, Young's modulus, and fracture toughness than those predicted by the rule of mixture for a coating in which the proportion of each material is equal to 50%. A significant presence of nitrogen atoms is identified in the vicinity of the interface, leading to a local modification of the chemical environment, and a swelling of the interface is also noticed. Interfaces with $TiAlN[111]_c$ exhibit better thermodynamic stability, whereas $TiAlN[200]_c$ interfaces display superior mechanical properties.