Investigation of the fracture mechanics in TiN thin films deposited on different substrates based on the digital material representation concept.

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Abstract

Titanium nitride (TiN) thin films are widely used materials for products with a high degree of biocompatibility and high strength resistance at the same time (e.g., implants). Therefore, TiN films are often used in implantology, from knee joint replacements to valve protection in the artificial human heart (1). However, electron and scanning electron microscopy analysis revealed the frequent occurrence of a complex columnar nanostructure in these materials resulting from the specific nature of the PLD (Pulsed Laser Deposition) (2) process. The morphology of such nanostructure is one of the main reasons for uncontrolled delamination and fracture observed in thin films under loading conditions. Accurate investigation of thin film fracture requires a series of very sophisticated laboratory experiments, which are time-consuming and expensive.
Therefore, this paper presents a new approach to the numerical analysis of crack evolution in TiN thin films deposited by PLD, taking into account the morphology of the thin film in an explicit manner with the digital material representation concept. The mechanical properties of the thin film and the substrate were determined with the nanoindentation tests conducted in laboratory conditions to provide flow stress models for numerical simulations. Then, the plugin for Abaqus software was implemented to generate 2D and 3D digital material representation models of the investigated thin film based on the microstructural characteristics. Finally, the crack propagation model was developed within the finite element method considering the cohesive type elements (CEs), eXtended Finite Element Method (XFEM) and brittle fracture criteria. The obtained numerical results were validated against a series of experimental data. The study proved that the model based on digital material representation (3) could be used for reliable predictions of local crack development in thin films deposited by the PLD method.

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