Hard Coatings and Vapor Deposition Technologies
Room Town & Country D - Session B4-2-MoA

Properties and Characterization of Hard Coatings and Surfaces II

Moderators: Naureen Ghafoor, Linköping University, Sweden, **Johan Nyman**, Linköping Univ., IFM, Thin Film Physics Div., Sweden, **Justinas Palisaitis**, Linköping Univ., IFM, Thin Film Physics Div., Sweden

1:40pm **B4-2-MoA-1 Microstructural Simulations on Thin Films***, **Vinzenz Guski (Vinzenz.Guski@imwf.uni-stuttgart.de)**, W. Verestek, S. Schmauder,* Universität Stuttgart, Germany **INVITED**

Due to their outstanding mechanical properties, hard coatings possess a wide range of applications as protective layers. However, an experimental determination of the properties of such thin coatings is not only difficult but also cost- and time intensive. In this regard, numerical methods, such as finite element method (FEM), have the ability to reduce the experimental effort, significantly. Usually, for characterisation of hard coatings indentation tests are performed to determine the hardness, the Young's modulus or the adhesive behaviour. With the aid of FE simulations, additional important effects such as residual stresses or the microstructure on the material properties can be investigated.

In the presented work FE simulations of indentation tests using a Vickers pyramid were carried out to investigate the mechanical behaviour of hard coatings in depth. During a sensitivity study, FE models with different coating microstructures, such as equiaxed or columnar grains with different grains size distributions, and coating thicknesses were established and analysed. Besides, the effect of residual stress on the mechanical behaviour are addressed. The performed simulations were validated by indentation test data and cross sections of the coatings. Finally, these simulation results deliver a property-microstructure-relation of the investigated hard coatings and can provide suggestions for optimization.

2:20pm **B4-2-MoA-3 Ab Initio Supported the Development of Tin/Mon Superlattice Thin Films With Improved Hardness and Toughness***, **Zecui Gao (zecui.gao@tuwien.ac.at)**, J. Buchinger, N. Koutná, T. Wojcik, R. Hahn, P. Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria

Motivated by superior strength and toughness indicators predicted for $TiN/MoN_{0.5}$ superlattices by ab initio calculations, we synthesize a series of TiN/MoN_y superlattice (SL) thin films by DC reactive magnetron sputtering to extract the superlattice effect on hardness and fracture toughness. The SLs crystallise with a single-phase centred cubic (fcc, rock salt) structure. The MoN_y layers are stabilised in their fcc structure by the coherent growth with TiN layers and low N_2-partial pressure, ensuring a close to $MoN_{0.5}$ stoichiometry, favouring fcc. Both hardness and toughness, reveal a distinct dependence on the bilayer period L, featuring a hardness peak of 34.8 ± 1.6 GPa for L = 9.5 nm. The fracture toughness (K_{IQ}) shows a significant enhancement compared to TiN (K_{IQ} ~ 2.2 MPa√m) and Mo_2N (K_{IQ} ~ 2.7 MPa√m) coatings, peaking with ~ 4.1 ± 0.3 MPa√m also at L = 9.5 nm.

2:40pm **B4-2-MoA-4 Effect of Substrate Bias on the Residual Stress Depth Profile and the Mechanical Properties of Ti-Al-N Coatings Prepared by Cathodic Arc Deposition***, **Luis Varela (luis-bernardo.varela-jimenez@polymtl.ca)**, K. Tsoutas, A. Miletic, E. Bousser,* Polytechnique Montréal, Canada*; J. Mendez,* MDS Coating Technologies Corporation, Canada*; J. Klemberg-Sapieha, L. Martinu,* Polytechnique Montréal, Canada

Ti-Al-N coatings were prepared by the Cathodic Arc Deposition (CAD) onto Inconel 718 substrates. The substrate bias voltage during deposition was varied, and we evaluated its effect on the residual stress (RS) distribution throughout the thickness of the coatings. Structural characterization and RS measurements were performed by classical X-ray Diffraction and synchrotron X-ray radiation measurements. Mechanical properties, namely the hardness and Young's modulus, were measured by depth-sensing indentation. The results indicate a higher compressive RS at the film surface (several GPa) that decays to a lower compressive stress value (hundreds of MPa) at the film/substrate interface. Hardness values significantly increased from 23 GPa to 31 GPa upon substrate bias increase, with a slight reduction of the Young's modulus. Similarly, the average compressive RS increased from 1.0 to 4.7 GPa for coatings deposited at bias voltages of 0V and -100V, respectively. As well, scanning electron microscopy morphological analysis of the cross-sections revealed a pronounced width reduction of the columns with the increase of the bias. The present findings provide a better insight into the impact of the substrate bias voltage on RS, film microstructure, and the mechanical properties of arc evaporated Ti-Al-N coatings. This allows one to select the most suitable coatings for specific mechanical solicitations in different industrial applications.

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