Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room San Diego - Session E2-1

Mechanical Properties and Adhesion

Moderators: Gerhard Dehm, Max-Planck Institut für Eisenforschung, Etienne Bousser, The University of Manchester, Fan-Bean Wu, National United University, Taiwan

1:50pm **E2-1-2 Cross-sectional Investigation of Microstructure and Mechanical Properties of Graded Ti(N,B) Coatings***, **Michael Tkadletz**, N Schalk, C Mitterer, C Hofer, J Keckes,* Montanuniversität Leoben, Austria*; M Deluca,* Materials Center Leoben Forschung GmbH, Austria*; M Pohler, C Czettl,* CERATIZIT Austria GmbH, Austria

Chemical vapor deposited (CVD) TiB_2 coatings are typically grown on a thin TiN base-layer to prevent diffusion of B into the substrate. While CVD TiN coatings exhibit a rather large grain size in the µm range, tensile residual stress and a relatively low hardness, the TiB_2 coatings are characterized by a nanocrystalline microstructure, high compressive residual stress and high hardness. In order to alleviate the resulting sharp transition at the interface of these two layers, an additional Ti(N,B) layer with B content gradually increasing from pure TiN to pure TiB_2 was introduced. Subsequently, the coating was investigated using scanning- as well as transmission electron microscopy, cross–sectional synchrotron X-ray nanodiffraction and cross–sectional dynamic nanoindentation and modulus mapping techniques. A grain size gradually decreasing from the µm to nm range, a significant change of residual stress from 0.5 to -2 GPa and an increase in hardness from ~18 to ~45 GPa with increasing B content could be observed across the coating thickness. With increasing B content, a transition from the face centered cubic to the hexagonal structure was also found. The formed compounds and their three dimensional arrangement was investigated by combinatorial use of Raman and X-ray photoelectron spectroscopy as well as atom probe tomography. The obtained results provide the basis for an evolutionary design of TiN/TiB_2 and Ti(B,N) coatings with optimized B content.

2:10pm **E2-1-3 Nanocrystalline Pt-Au MEMS Electrical Switches***, **Nicolas Argibay**, M Dugger, D Adams, C Nordquist, A Grine, M Henry, P Lu,* Sandia National Laboratories, USA

Microelectromechanical systems (MEMS) relays have orders of magnitude higher figure of merit compared to semiconductor devices, along with lower power consumption and insertion loss. Unfortunately, MEMS switches have not penetrated high volume applications partly due to contact adhesion, contamination, high cycle switch life and microstructural evolution leading to performance drift.

Recent work has shown that it is possible to achieve extraordinarily stable nanocrystallinity in some binary metal alloys via solute segregation in the as-deposited state, even at high temperatures. One of these alloys, Pt-Au, may provide solutions to several challenges preventing greater adoption of MEMS switches. As-deposited nanocrystalline Pt grains are stabilized by the presence of Au at grain boundaries, presenting the possibility of reduced creep and relaxation in the electrical contacts and structural elements of a MEMS switch. Sputtered Pt-Au was used to construct MEMS switches, and initial results suggest performance improvements relative to baseline switches made from Au. MEMS switch performance and associated material evolution mechanisms will be discussed.

2:30pm **E2-1-4 Thin Film Metallic Glass: Novel Coating Providing High Toughness and Low Friction***, **Chia-Chi Yu**, J Chu,* National Taiwan University of Science and Technology, Taiwan*; Y Shen,* University of New Mexico, USA

The amorphous nature of thin film metallic glasses (TFMGs) provides outstanding mechanical properties, including high strength, large elastic limits, and excellent corrosion and wear resistance. The grain boundary-free structure of TFMGs produces an exceptionally smooth surface and low surface free energy, resulting in high hydrophobicity and a low coefficient of friction.

In this study, magnetron sputtering was used in the deposition of Zr-based TFMG coatings with the aim of enhancing the bending and fatigue properties of bulk metallic glasses (BMGs). A TFMG coating was shown to increase the plastic strain of BMG by 9.2%, without sacrificing its extraordinary strength. This was also shown to increase the fatigue endurance-limit of BMG by ~33%, from 300 MPa for bare BMG to 400 MPa for TFMG-coated BMG. The results of transmission electron microscopy and nanoindentation testing revealed that TFMGs are able to withstand enormous shear strain without fracturing. Used as a coating on syringe needles, the low coefficient of friction of TFMG (∼0.05) reduced the insertion forces by ∼66% and retraction forces by ∼72%, when tested on polyurethane rubber blocks.

2:50pm **E2-1-5 Driving Force for the Texture Transformation of Thin Metal Films***, E Ellis,* Cornell University, USA*; M Chmielus,* University of Pittsburgh, USA*; S Baker,* Cornell University, USA*; Y Cheng, P Liu, **Ming-Tzer Lin**,* National Chung Hsing University, Taiwan **INVITED**

The texture transformation has been attributed to a competition between strain energy and interface energy. In FCC materials, the (111) orientation has the lowest interface energy, while the (100) orientation has the lowest biaxial modulus. Thus, at a given strain, the interface energy per unit volume decreases as the inverse of the film thickness, while the strain energy per unit volume is constant with film thickness. However, recent studies have questioned the role of both stresses and interface energies in this texture transformation. Where stresses are known with certainty, they have been shown to be insufficient to produce the texture transition, and the transitions seem to occur in films of similar thickness regardless of the interface conditions. We simulated the driving forces using a first principle density functional theory for the orientation selection mechanisms and investigated the transformation by using a bulge test apparatus to induce different stresses in thin Ag films under identical annealing conditions. *In situ* synchrotron XRD measurements show the change in texture during annealing, and reveal that applied stresses have no effect on the transformation. Stress analysis shows that differences in driving forces for texture transformation due to applied bulge pressure were significant ($\approx$200 kJ/m^3), suggesting that a different, much larger driving force must be responsible. Reduction in defect energy has been proposed as an alternative. However, vacancy and dislocation densities must be exceptionally high to significantly exceed the strain energy and do not provide obvious orientation selection mechanisms. Nanotwins in reported densities are shown to provide greater driving force ($\approx$ 1000 kJ/m^3) and may account for orientation selection. The large difference between the calculated strain and defect energies and the driving force for grain growth (21,100 kJ/m^3) casts doubt on the applicability of a thermodynamic model of texture transformation.

3:30pm **E2-1-7 Strength and Strain Hardening Behavior of Particle Strengthened Coherent Cu/Ni Multilayer Films***, **Rachel Schoeppner**, M Polyakov, G Mohanty, J Michler,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

There are many techniques used to increase the strength of a material depending on the application and desired results. Two such techniques include deposition of nanolaminate structures and the addition of hard particles to act as dislocation barriers. Particles have been known to act as barriers to dislocation motion as well as Frank-Read dislocation sources, which both increases the strength and strain-hardening ability of the material. This type of strengthening has traditionally only been applied to bulk alloys and oxide dispersion strengthened materials with no investigations focusing on the combined affect of particles distributed at the interface of nanoscale multilayer films. Some molecular dynamic simulations focusing on steps and imperfections specifically at the interface of Cu/Nb multilayer films have shown additional strengthening can occur as the step size of the kink increases; however, the presence of these interfacial defects can also result in an initial decrease of the yield strength as they act as dislocation sources, initiating plasticity sooner than in films with pristine interfaces, which is similar to the concept of Frank-Read sources in traditional particle strengthened films. The extent of the interaction of hard W nanoparticles deposited at the usually coherent interface of Cu/Ni multilayer films has been investigated through both nanoindentation and micropillar compression to determine both the strengthening and strain-hardening affect of these particle enforced interfaces. Initial investigations have shown an overall increase in the nanoindentation hardness of these films by a maximum of 1 GPa when compared to CuNi multilayers without particles at the interface. However, as the particle density increases the amount of strengthening is actually shown to decrease in the range of volume fractions investigated here. Further microstructural and mechanical characterizations have also been conducted to more fully explain this phenomenon.

3:50pm **E2-1-8 Indentation Induced Deformation and Damage in Metal-Ceramic Multilayer Coatings**, ***Yu-Lin Shen***, *R Jamison,* University of New Mexico, USA

Metal-ceramic multilayer composite coatings are an exciting subset of materials with many promising attributes. This presentation highlights our recent studies on mechanical characterization of such coatings using the nanoindentation technique. We focus on aluminum (Al)/silicon carbide (SiC) nanolayers, which serves as a model system for investigating the constraining effect due to the highly mismatched mechanical properties of the constituents. How this structural heterogeneity can affect the indentation behavior is a current a subject of active research. The development of complex deformation patterns underneath the indentation, dictated by the structural heterogeneity, can lead to various forms of local damage. Our studies focus on the employment of numerical finite element modeling to corroborate with experimental observations as well as to extract meaningful constitutive properties. Special attention is given to the analyses of (i) plastic deformation in the metal layers, (ii) cyclic indentation response and composite modulus measurement and (iii) indentation-induced delamination.

4:10pm **E2-1-9 Influence of Various Interlayers on Mechanical Properties of CrAlN Coatings on Tungsten Carbide Substrate**, ***HoeKun Kim***, *J La, M Song, S Lee, Y Hong,* Korea Aerospace University, Republic of Korea

Among many ternary nitride protective coatings, the CrAlN coatings have been paid much attention to the cutting tool's coating applications due to their excellent properties such as high hardness, low surface roughness, and excellent thermal stability. It was reported that the interlayer with the median hardness to elastic modulus ratio (H/E ratio) between the value of the coating and the substrate improved the wear resistance of the coating. In this work, various interlayers such as CrN, CrZrN, CrN/CrZrSiN were synthesized between the CrAlN coating and the tungsten carbide substrate to improve mechanical properties of the coatings. All the coatings were produced by an unbalanced magnetron sputtering system on the WC-6 wt.% Co substrate, and total thickness was controlled to be 3 µm. The microstructure, hardness and elastic modulus, and friction coefficient were evaluated by field-emission scanning electron microscopy (FE-SEM), nano-indentation, and ball-on-disc type wear tester, respectively. All the coatings were annealed at temperatures from 600 to 1000˚C in furnace for 30 min, and the hardness values were investigated using nano-indentation.

The hardness and elastic modulus of all the CrAlN coatings were not affected significantly by type of the interlayer, and they were measured to be in the ranges of 35.5 to 36.2 GPa and 424.3 to 429.2 GPa, respectively. However, wear test showed that the CrAlN coatings with the CrN and CrN/CrZrN interlayer exhibited improved friction coefficient of 0.34 compared to the CrAlN coating with the CrZrN interlayer (COF 0.41), and the wear rate and width of those coatings showed lower values. These improved wear properties could be attributed to the H/E ratio of the interlayer between the CrAlN coating and the WC substrate. In view of the coating structure, there exists a gradual decrease in the H/E ratio from the CrAlN coating (H/E, 0.089), to the CrZrSiN interlayer (H/E, 0.083) and CrN interlayer (H/E, 0.076), and the WC substrate (H/E, 0.040). The CrZrSiN and CrN interlayers induced a smooth transition of the stress effectively under loading conditions during the wear test, and this led improved wear resistance of the CrAlN coating. During the thermal stability tests, the hardness of the CrAlN coating with the CrN/CrZrSiN coating was maintained up to 1000˚C due to excellent oxidation resistance of the CrZrSiN layer consist of the amorphous SiN phase .

4:30pm **E2-1-10 Numerical Investigation of Damage and Fracture in Hard Nano-coating Layers using Cohesive Zone Modeling**, ***Shahed Rezaei***, *S Wulfinghoff, S Reese,* RWTH Aachen University, Germany

Coating layers are usually applied on different manufacturing tools in, e.g., plastic extruder in order to increase their lifetime and to improve the surface properties of the final parts. New coating deposition techniques such as high-power impulse magnetron sputtering (HPPMS) can provide more parameters to control the coating mechanical properties, therefore they result in producing coating layers with better performance and perhaps higher damage resistance. In order to be able to compare the effect of different parameters on damage behaviour of the coatings, a cohesive zone (CZ) element model has been applied. The fracture modes are divided into an intergranular fracture inside the coating and delamination between the coating layer and the substrate. The developed numerical model allows predicting the damage initiation and propagation within various types of coating systems in different setups such as nanoindentation. Numerical studies of nanoindentation tests show that the intergranular cohesive tractions, residual stresses, elastic and plastic properties and the grain morphology of the coating layers are the most effective parameters in order to produce stronger coatings.

Author Index

Bold page numbers indicate presenter