Hard Coatings and Vapor Deposition Technologies
Room California - Session B5-1-ThA

Hard and Multifunctional Nanostructured Coatings I

Moderators: Tomas Kozak, University of West Bohemia, **Helmut Riedl**, TU Wien, Institute of Materials Science and Technology

2:00pm **B5-1-ThA-3 Interfaces and Mechanisms: A Molecular Dynamics Approach to Fine Tuning Manipulation of Mechanical Properties**, ***Alberto Fraile***, *H Yavas, E Frutos,* Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Czech Republic*; T Huminiuc,* Engineering Science, Faculty of Engineering and the Environment, University of Southampton, Southampton, UK*; T Polcar,* Czech Technical University in Prague, Czech Republic

With the advent of more and more powerful supercomputers, Molecular Dynamics (MD) is playing today a capital role in the understanding of the deformation mechanisms at the atomic scale of all kind of materials under different scenarios. Many investigations have demonstrated that the peculiar features of nanoplasticity generated during indentation can be analyzed in detail by this technique.

Using MD we are constructing deformation-mechanism maps based on fundamental physical processes in the deformation of nanostructured materials. The knowledge for these processes comes from modelling the nanostructures at the atomic level by using atomistic simulations. The power of our approach is that it integrates the most important physics associated with deformation phenomena, in a self-consistent description of the effects of stress, interfaces and grain size on the mechanical properties in nanocrystalline structures, thereby avoiding the empiricism of other methods.

We have prepared different Zr/Nb layered systems (with different Nb/Zr geometries and/or structures) and indentation hardness close to the theoretical limits was measured for special cases. Then, our theoretical calculations were compared to the experimental results. Special attention was devoted to the effect of interlayers, grain boundaries, dislocation reactions as well as the effect of phase transitions in Zr.

The dominant deformation mechanism of metallic multilayered systems is the confined volume dislocation reactions, however, we also showed that there is a high possibility to control the deformation by tunning phase transformations at the nanoscale. This knowledge will open new doors to shed light into hidden features of the deformation and strengthening mechanisms guiding the design the next generation of metallic coatings and alloys.

2:20pm **B5-1-ThA-4 Preparation of Hard Yet Fracture Resistant W-B-C Coatings Using High Power Impulse Magnetron Sputtering**, ***Pavel Soucek***, *M Polacek, P Klein, L Zabransky, V Bursikova, M Stupavska,* Masaryk University, Brno, Czech Republic*; Z Czigany, K Balazsi,* Hungarian Academy of Sciences, Hungary*; P Vasina,* Masaryk University, Brno, Czech Republic

As the demands for the quality and speed of machining increase, the application of protective coatings on the used cutting tools becomes ever more important. Nowadays used ceramic protective coatings exhibit high hardness and toughness, however, they suffer from inherent brittleness. This can lead to a premature failure of the coating and of therefore of the cutting tool as a whole due to rapid crack propagation. Thus, a new generation of coatings combining hardness and moderate ductility is sought for.

Such a combination of seemingly mutually exclusive properties was recently predicted by ab-initio calculations in inherently nanolaminated X_2BC crystalline coatings, where X is a metallic element [1]. W_2BC system was found the most promising regarding its mechanical properties with predicted Young's modulus of ~ 470 GPa, B/G ratio of 1.91 and Cauchy pressure of 71 GPa. However, only a near zero negative value of its formation enthalpy of -0.16 eV/atom predicts problems with crystallization of this phase [1]. Indeed, previous works using mid-frequency pulsed DC sputtering did not report the formation of the crystalline W_2BC phase [2].

This contribution reports on the synthesis and comparison of W-B-C coatings sputtered from a compound W_2BC target using DCMS and HiPIMS, respectively. Different substrate temperatures up to 700°C were used in each case. The differences in the DCMS and HiPIMS deposition processes will be discussed. The microstructure of the coatings is investigated and is correlated to their mechanical properties. The fracture resistance and the deformation behaviour of the coatings will be discussed. Simultaneous achievement of high hardness and fracture resistance will be shown as well as the means of its achievement will be discussed.

This research has been supported by project LO1411 (NPU I) funded by the Ministry of Education, Youth and Sports of the Czech Republic.

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2:40pm **B5-1-ThA-5 Analytical Modelling of Misfit Dislocation Formation in Superlattice Coatings and its Effect on the Fracture Toughness**, ***Antonia Wagner***, TU Wien, Institute of Materials Science and Technology, Austria*; D Holec,* Montanuniversität Leoben, Austria*; M Todt,* TU Wien, Institute of Lightweight Design and Structural Biomechanics, Austria*; P Mayrhofer, M Bartosik,* TU Wien, Institute of Materials Science and Technology, Austria

Coherently grown multilayer coatings with a bilayer period in the nanometer range exhibit a superlattice (SL) effect in mechanical properties like hardness and fracture toughness [1, 2]. While the superlattice effect in hardness is well described by the model after Chu and Barnett [3] based on dislocation plasticity, the fracture toughness enhancement in 'all-ceramic' SL coatings is not primarily governed by plasticity and the underlying mechanisms are less well understood.

The aim of the present work is to study the effect of the residual stress state in SL coatings on the fracture toughness. In general, extrinsic residual stresses (due to a mismatch of the coefficients of thermal expansion) and intrinsic stresses (stemming from the film growth process) contribute to the overall stress state. A major part of the intrinsic stresses, in turn, are coherency stresses, which originate from the epitaxial growth and the lattice mismatch of the film forming phases and the substrate material. While the thermal mismatch stresses are almost independent of the individual layer thicknesses, coherency stresses show a strong dependency when considering the formation of misfit dislocations. Up to a critical thickness of the layers, the misfit in the lattice parameters is accommodated by elastic strain, thereafter misfit dislocations form, preferably at the interface to the substrate or the previously deposited layer [4, 5].

We have calculated the dislocation density as a function of the layer thickness by an energy balance considering the strain energy of the system and the dislocation energy. An analytical model - with layerwise deposition of the individual layers including misfit dislocations - was developed to predict the stress state of superlattice systems as a function of the bilayer period. Finally, the fracture toughness and its dependence on the bilayer period was calculated taking into account the stress state, the intrinsic fracture toughness of the phases and the spatial variation of elastic properties of respective SL architectures.

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3:00pm **B5-1-ThA-6 The Electrical Response of PVD Deposited Nanocrystallited Carbon Film in Magnetic Field**, ***Chao Wang***, *J Guo, X Dai,* Institute of Nanosurface Science and Engineering, College of Mechatronics and Control Engineering, Shenzhen University, China

Nano-crystallited carbon film has gained much attentions due to its excellent electrical and mechanical properties, especially its magnetoresistance (MR) at room temperature. The novel electrical response of this film under external magnetic field shed light on a new-type carbon based magnetic sensing device. Recently, it is found that the MR performances of the film can be strongly improved by introducing Si as substrate instead of SiO 2 . Transport study implied that the film has high carrier density and ultra low mobility, which may be originated from the modulation effect of n-type doping substrate.

In this study, nanocrystallited carbon films were deposited on silica and N-type silicon substartes with plasma assisted PVD method. The nanocrystallited structure were observed through high resolution TEM and

Raman spectra. The change of electrical resistances along with temperature and magnetic field strength were measured by using Quantum Design physical property measurement system(PPMS). The results showed that the nanocrystallied films showed large magnetoresistance at 300K, which is favorable for room temperature applications. The magnetic response behavior of the carbon films on different substrates were compared, which suggested that the n-silicon substrate can remarkably improved the magnetoresistacnce coefficient. The influences of gas flow, bias voltage, and deposition time on the structure, carrier density and magnetoresistance of the carbon films were invesitgated, and the transport mechanism of carriers in the films were discussed. We also found the large magnetoresistance of the film when using alternating current as stimulating source, when the largest rate of magnetoresistance can reach to 1000% per tesla at room temperature. This is ascribled to the inductive as well as spin-enhanced magnetoresistance effect due to the oriented graphene nanocrystalltes inside the semiconductive film matrix.

3:20pm **B5-1-ThA-7 Aluminium Nitride Based Piezoelectric MEMS: From Material Aspects to Low Power Devices***, **Ulrich Schmid**, M Schneider,* TU Wien - Institute of Sensor and Actuator Systems, Austria **INVITED**

In a compact introduction, I will motivate the benefits of piezoelectric thin films for MEMS and will give a short overview to state of art application scenarios on device level. Next, I will highlight latest results on the electrical, mechanical and piezoelectrical characterization of sputter-deposited aluminium nitride (AlN) including the impact of sputter parameters, film thickness and substrate pre-conditioning [1,2]. I will present the impact of doping of AlN with scandium, which leads to an increase of the moderate piezoelectric coefficient of AlN up to a factor of four. In a next step, these films are implemented into fabrication processes of cantilever-type MEMS devices. In combination with a tailored electrode design, resonators are realized featuring Q factors up to about 300 in liquids covering the frequency range of 1-2 MHz. This enables the precise determination of the viscosity and density of fluids up to dynamic viscosity values of almost 300 mPas [3]. Besides this application, such high Q factors are useful when targeting mass-sensitive sensors, thus paving the way to e.g. particle detection even in highly viscous media. Given the low increase in permittivity of ScAlN compared to AlN, another field of application for this material are vibrational energy harvesters, where the benefit of ScAlN compared to pure AlN is demonstrated [4]. Finally, I will present some selected results of ScAlN thin films within SAW devices ranging from high temperature applications to droplet manipulation in microfluidics [5].

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4:00pm **B5-1-ThA-9 Superamphiphobic Surface Produced by Femtosecond Laser Patterning and Pulsed Plasma Polymerization***, **Cheng-Wei Lin,*** Feng Chia University; Central Taiwan University of Science and Technology, Taiwan*; G Lu, X Chang, P Hsieh,* Feng Chia University, Taiwan*; C Chou,* Department of Surgery, Taichung Veterans General Hospital, National Yang-Ming University, Taiwan*; C Chung,* Central Taiwan University of Science and Technology, Taiwan*; J He,* Feng Chia University, Taiwan

The superamphiphobic surface may be widely applied, including medical devices, kitchen wares, architectures, and automotives, but is a challenging technique, with the unique characteristics of water and low surface tension liquids repelling, self-cleaning, anti-freezing and anti-bacterial activity. In this study, a dual-technique of surface modification by employing femtosecond laser patterning and pulsed plasma polymerization of octafluorocyclobutane was used to develop a superamphiphobic surface on the AISI 304 stainless steel substrate. Experimental results showed that the treated surfaces exhibited high water and oil contact angle, which may be attributed to nano/micro surface structure and low-surface-energy of fluorocarbon coating, as identified by SEM and FTIR analysis. In the steel wool scratch test, the superamphiphobic surface showed high mechanical durability even under harsh conditions. This indicates that such technique may have the potential in regulating surface properties of medical devices for different purposes.

Author Index

Bold page numbers indicate presenter

— B —
Balazsi, K: B5-1-ThA-4, 1
Bartosik, M: B5-1-ThA-5, 1
Bursikova, V: B5-1-ThA-4, 1
— C —
Chang, X: B5-1-ThA-9, 2
Chou, C: B5-1-ThA-9, 2
Chung, C: B5-1-ThA-9, 2
Czigany, Z: B5-1-ThA-4, 1
— D —
Dai, X: B5-1-ThA-6, 1
— F —
Fraile, A: B5-1-ThA-3, **1**
Frutos, E: B5-1-ThA-3, 1
— G —
Guo, J: B5-1-ThA-6, 1
— H —
He, J: B5-1-ThA-9, 2
Holec, D: B5-1-ThA-5, 1
Hsieh, P: B5-1-ThA-9, 2
Huminiuc, T: B5-1-ThA-3, 1
— K —
Klein, P: B5-1-ThA-4, 1
— L —
Lin, C: B5-1-ThA-9, **2**
Lu, G: B5-1-ThA-9, 2
— M —
Mayrhofer, P: B5-1-ThA-5, 1
— P —
Polacek, M: B5-1-ThA-4, 1
Polcar, T: B5-1-ThA-3, 1
— S —
Schmid, U: B5-1-ThA-7, **2**
Schneider, M: B5-1-ThA-7, 2
Soucek, P: B5-1-ThA-4, **1**
Stupavska, M: B5-1-ThA-4, 1
— T —
Todt, M: B5-1-ThA-5, 1
— V —
Vasina, P: B5-1-ThA-4, 1
— W —
Wagner, A: B5-1-ThA-5, **1**
Wang, C: B5-1-ThA-6, **1**
— Y —
Yavas, H: B5-1-ThA-3, 1
— Z —
Zabransky, L: B5-1-ThA-4, 1