New Horizons in Coatings and Thin Films
Room Pacific D - Session F4-1-WeM

New Horizons in Boron-Containing Coatings I

Moderators: Helmut Riedl, TU Wien, Austria, **Johanna Rosén**, Linköping University, Sweden

8:00am **F4-1-WeM-1 Synthesis and Oxidation Behavior of $Ti_{0.35}Al_{0.65}B_y$(y= 1.69- 2.43) Coatings***, A. Navidi Kashani, S. Mráz, D. Holzapfel, M. Hans,* RWTH Aachen University, Germany*; D. Primetzhofer,* Uppsala University, Sweden*; L. Löfler, P. Ondracka,* ***Jochen Schneider (schneider@mch.rwth-aachen.de),*** RWTH Aachen University, Germany

The effect of B concentration on the phase formation and oxidation resistance of $(Ti_{0.35}Al_{0.65})$By with y = 1.69, 2.03, 2.43 coatings was investigated. Elemental B targets in radio frequency (RF) mode and a compound $Ti_{0.4}Al_{0.6}$ target in direct current (DC) mode at floating potential were sputtered. The B concentration was varied systematically by adjusting the applied power to the respective magnetrons while keeping the power supplied to the magnetron with the $Ti_{0.4}Al_{0.6}$ target constant. The oxidation resistance at 700 °C in air for up to 8 hours was compared to a cathodic arc evaporated $(Ti_{0.37}Al_{0.63})_{0.49}N_{0.51}$ coating with an Al/Ti ratio of 1.69 ± 0.19 which is very similar to 1.84 ± 0.42 for the boride coatings. Scanning transmission electron microscopy (STEM) imaging revealed oxide scale thicknesses of 39 ± 7 and 101 ± 25 nm for $(Ti_{0.35}Al_{0.65})B_{2.03}$ and $(Ti_{0.37}Al_{0.63})_{0.49}N_{0.51}$ after 8 hours, respectively. Hence, the close to stoichiometric boride outperforms the nitride coating. This behavior can be understood based on compositional and structural analysis of the oxide scales: While the oxide layer on the diboride is primarily composed of Al and O and protective, the oxide layer on the nitride coating is porous and contains Ti, Al and O.

8:20am **F4-1-WeM-2 Influence of Si Alloying on the High-Temperature Mechanical Properties of CrB_2 Based Thin Films***,* ***Lukas Zauner (lukas.zauner@tuwien.ac.at)****, T. Glechner, R. Hahn,* Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria*; O. Hunold, J. Ramm,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; P. Polcik,* Plansee Composite Materials GmbH, Germany*; H. Riedl,* Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria

Among transition-metal diboride based thin films CrB_2 is an exciting prospect due to a unique portfolio of materials properties, especially through offering high fracture resistance [1]. However, this class of PVD coatings suffers from an inherently low oxidation resistance. Therefore, establishing pathways to improve the oxidation resistance and thus maintain the mechanical properties to higher temperatures (*i.e.*, above 1000 °C) for these hard-protective coatings is an integral aspect for future high-performance components in thermo-mechanically demanding environments.

In this work, the influence of Si alloying on the high-temperature mechanical properties and fracture toughness of magnetron sputtered CrB_2 thin films is studied for various concentrations. As indicated by thermogravimetric analysis, adding Si to the hexagonal α-AlB_2 structured coatings improves the onset of oxidation by at least 600 °C in lab-air conditions. This drastic improvement in the formation of a stable oxide scale is further correlated with detailed analysis on the thermal stability and phase formation as obtained by non-ambient X-ray diffraction in both vacuum and lab-air atmospheres. The mechanical properties of the synthesised Cr-Si-$B_{2\pm z}$ thin films – including hardness, Young's modulus and fracture toughness – are obtained by nanoindentation and bending of pre-notched, unstrained micro-cantilever beams in the as-deposited as well as the annealed state. Complementary in-situ characterisation of the aforementioned mechanical properties on coated high temperature bulk materials up to 800 °C allowed for a direct identification of changes in the deformation and fracture mechanisms across the investigated temperature regime [2]. Hence, this study showcases the potential of transition-metal diboride thin films – a class previously deemed unsuitable for high-temperature applications – by utilising Si-alloying to preserve the CrB_2 thin films.

[1] Gu, Xinlei, et al. "Sorting transition-metal diborides: New descriptor for mechanical properties." *Acta Materialia* 207 (2021): 116685.

[2] Buchinger, J., et al. "Fracture properties of thin film TiN at elevated temperatures." *Materials & Design* 194 (2020): 108885.

8:40am **F4-1-WeM-3 Design of Novel Transition Metal Diboride-Based Pvd Thin Films: From Pure Compounds to Alloys, Composites and Multilayers***,* ***Michael Stueber (michael.stueber@kit.edu)****, V. Ott, S. Ulrich,* Karlsruhe Institute of Technology (KIT), Germany*; H. Riedl, P. Mayrhofer,* Technische Universität Wien, Austria **INVITED**

Transition metal diboride hard coatings are attractive material candidates for various high performance applications in engineering. Due to their chemical nature and microstructure these materials exhibit interesting multifunctional properties. Unfortunately, their mechanical properties (i.e. toughness and ductility) and the demand for achieving stoichiometric film composition or appropriate adhesion onto various substrates in physical vapor deposition processes make their utilization often a challenge. Thus, such materials and their deposition experience currently a strong revitalization of research efforts. This presentation will review the recent status of PVD transition metal diboride-based thin films, with a focus on magnetron sputtering techniques. It includes a brief retrospect on pioneering developments in the field, covering fundamental materials science aspects of the diborides as well as advanced coating design concepts such as the various Ti-B-C-N thin films. The major part of the presentation will discuss three design concepts for novel boride-based hard and tough coatings for engineering applications. These are mainly based on the model thin film material TiB_2 which is by far the most detailed characterized PVD transition metal diboride. The first approach describes the alloying of TiB_2 with the intention to design ternary solid solutions, $(Ti,X)B_2$ where X is another metal such as Al, Cr, Zr, V or others. The impact of Al content on phase formation, microstructure and mechanical properties of magnetron-sputtered $(Ti,Al)B_2$ thin films will be described. A second approach refers on the formation of TiB_2-metal composite thin films, which covers the objectives of designing thin film material composed either of a boride matrix with dispersed metal nanoclusters or of a metal matrix with dispersed diboride cluster phase. The metal phase used in this part of the description is the superalloy B2 structured NiAl. Phase formation and microstructure evolution of magnetron co-sputtered TiB_2-NiAl thin films will be covered, both in as-deposited and vacuum annealed state. The third approach deals with the integration of TiB_2 layers into nanoscale multilayers when the second layer constituent is also a metal layer. Focus is again on the combination of TiB_2 with NiAl. Multilayers with variation of the bilayer period and its impact on their structure and properties will be considered. Other relevant diboride thin film design concepts and newest progress achieved by advanced PVD techniques such as HIPIMS or hybrid PVD processes will also be reported.

9:20am **F4-1-WeM-5 Tribological Properties and Thermal Stability of $V_{1-x}Mo_xB_y$ Coatings***,* ***Katarína Viskupová (katarina.viskupova@fmph.uniba.sk)****, B. Grančič, T. Roch, M. Truchlý, M. Mikula, V. Šroba, L. Satrapinskyy, P. Kúš,* Comenius University, Bratislava, Slovakia

Development of space technology encourages research of new materials that are highly performing in extreme conditions. An important category are low wear resistance solid lubricants with stable properties at temperatures above 1000°C and in oxidative environments. Currently widely studied transition metal diborides (TMB_2) offer high temperature stability and excellent mechanical properties, such as high hardness and wear resistance. Vanadium diboride also shows promising tribological properties due to lubrication effect of oxidation products B_2O_3 and V_2O_5 [1]. Our aim is to study effects of alloying of VB_2 coatings with Mo, which may lead to structural decomposition and hence provide good mechanical properties at high temperatures [2]. Moreover, possible formation of MoO_3 during oxidation may influence the tribological properties of the coatings [3]. In our work, we use physical vapour deposition for preparation of $V_{1-x}Mo_xB_y$ films with different Mo concentration and B/TM ratio. We discuss the relationship between chemical composition, structure formation and structure evolution during vacuum annealing up to 1300°C. We further investigate the influence on hardness, elastic modulus, and friction coefficient at elevated temperature in air. Our results are supported by density functional theory calculations.

[1] A. Erdemir et al., Wear 205 (1997) 236-239

[2] B. Alling et al., Scientific Reports 5 (2015) 9888

[3] W. Gulbiński et al., Wear 254 (2003) 129–135

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