Hard Coatings and Vapor Deposition Technologies
Room Town & Country C - Session B6-1-WeM

Coating Design and Architectures I

Moderator: Paul Heinz Mayrhofer, Institute of Materials Science and Technology, TU Wien, Austria

11:00am **B6-1-WeM-10 Thermally Induced Phase Formation in Magnetron Sputtered Ru/Al Multilayers - Impact of Modulation Period on Transition Temperatures and Phase Sequence***, Vincent Ott (vincent.ott@kit.edu),* Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany*; C. Schaefer,* Saarland University, Chair of Functional Materials, Germany*; T. Weingaertner, S. Ulrich,* Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany*; C. Pauly,* Saarland University, Chair of Functional Materials, Germany*; M. Stueber,* Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany

Intermetallic phases in the CsCl B2 structure like NiAl are in focus since long as engineering materials for high temperature applications. Besides good thermal conductivity, they offer high melting points and good oxidation resistance. A major disadvantage is its brittleness, which limits not only its processing at room temperature but also its potential applications. A promising candidate material with improved mechanical properties is the B2 RuAl phase.

Nanoscale multilayer coatings, which can exhibit self-propagating reactions, are a promising approach to synthesize coatings with a targeted microstructure that allows to tailor the material properties. We will show that the synthesis of B2 structured RuAl thin films is also possible by thermal activation close to equilibrium conditions without ignition of the exothermic self-propagating reaction by utilizing a imprinted nanoscale thin film architecture.It will be demonstrated for magnetron-sputtered Ru/Al multilayer thin films, that a specific phase formation sequenceis dependent of the modulation length and microstructure of the bilayers.Thus, by controlling the phase formation sequence, the microstructure of the resulting single-phase AlRu layer can be tuned. For a specific nanoscale layer design, the final phase AlRu can be formed directly from the deposited multilayer state via this approach, without the formation of intermediate intermetallic phases. This statement will be supported by in-situ HT-XRD, TEM, AES mapping and further analyses.

11:20am **B6-1-WeM-11 Structural Design of Diboride Thin Films (Virtual Presentation)***, Marian Mikula (mikula@fmph.uniba.sk),* *T. Fiantok,* Comenius University in Bratislava, Slovakia*; N. Koutná,* Linkoping University, Sweden*; V. Šroba,* Comenius University in Bratislava, Slovakia*; D. Sangiovanni,* Linkoping University, Sweden **INVITED**

Transition metal diborides from the group IIIB to VIIB (TMB_2) represent promising candidates for hard and protective films applicable in extreme temperature conditions and under high mechanical loads. This idea is motivated by the knowledge of their bulk equivalents which exhibit excellent mechanical properties, chemical inertness, high temperature stability and good oxidation resistance. Physical vapor deposition (PVD) techniques allow the growth of TMB_2 films with a specific nanocomposite character often formed by (sub)stoichiometric crystalline α-TMB_2/ω-TMB_2 nanofilaments embedded in an amorphous matrix. Although, these films are extremely hard, unfortunately, they are also inherently brittle, and the presence of an amorphous matrix provides an easy pathway for undesired oxidation at relatively low temperatures. For this reason, their application potential is currently very limited and suitable improvements to their weaknesses are intensively sought: (i) from a technological view, it is the use of progressive technologies (HiPPMS, HiTUS) and understanding the relationship between deposition parameters and specific diboride growth; (ii) from a structural point of view, it is the concept of alloying and multilayer architecture where a certain "tuning" of the films could lead to an improvement of the high-temperature behavior and a more ductile response to the mechanical load. Transport of Ions in Matter simulations and Time-resolved Mass Spectroscopy of deposition processes are very useful tools where we can better understand the growth of diboride films. Here, different angular distribution, ionization of target species, influence of Ar neutrals play an important role. Furthermore, using Density Functional Theory calculations we can predict the structural evolution of diboride systems, and their mechanical properties based on thermodynamic assumptions and valence electron concentrations. As we will show, the simplistic models used in DFT calculations at 0 kelvin are unable to predict formation of nanocomposite structures in diboride films, which are more complex in comparison to, e.g., single phase TM nitride films. In this lecture, several case studies of diboride films will be discussed, with the main focus on improving their mechanical and physical properties using a combination of theoretical predictions and experimental approaches.

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