MM 19: Topical Session: Combinatorial Materials Science I

Time: Tuesday 10:15–11:30 Location: H25

Topical Talk MM 19.1 Tue 10:15 H25

Development of new materials using high-throughput thin film experimentation and up-scaling — •Alfred Ludwig — Ruhr-Universität Bochum, Germany

New or optimized multifunctional materials are needed, e.g. for miniaturization of technological products with improved functionality even in extreme conditions or for efficient production/storage/conversion of energy carriers. For the discovery and optimization of new materials combinatorial and high-throughput experimentation methods are very effective. The materials to be investigated are deposited in the form of materials libraries by special magnetron sputter deposition methods (co-deposition, wedge-type multilayer deposition, shadow masking). These materials libraries are subsequently processed and characterized by high-throughput experimentation methods (automated EDX, XRD, temperature-dependent resistance and stress screening) in order to relate compositional information with structural and functional properties. The talk will cover examples of the combinatorial development of intermetallic materials for shape memory (Ni-Ti-X-Y, Fe-Pd-X) applications as well as new materials for solar water splitting. The obtained results are visualized in the form of composition-function diagrams. Examples of up-scaling from thin film findings to bulk applications are discussed.

Topical Talk MM 19.2 Tue 10:45 H25

A combinatorial approach to the synthesis of novel oxide and oxinitride thin films — •Michael Stüber, Stefanie Spitz, Harald Leiste, and Sven Ulrich — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-AWP), 76344 Eggenstein-Leopoldshafen, Germany

The development of new oxide and oxinitride thin films for engineering applications is attracting enormous interest. Besides theoretical modelling of structural design and properties of such materials the systematic evaluation of plasma-based deposition routes towards their synthesis will contribute to create a substantial data base for future material development.

An experimental combinatorial approach to the synthesis of oxide and oxinitride thin films in the systems Al-Cr-O-N and Cr-Zr-O-N will be presented. The thin films were deposited by reactive r.f. magnetron sputtering at 500 °C and 500 W r.f. target power under systematic variation of the reactive gas flows. Thin films with five different compositions were obtained in one deposition process by using a segmented Al:Cr or Cr:Zr sputtering target.

Under specific conditions, (Al,Cr)2O3, (Cr,Zr)2O3, (Al,Cr)2(O,N)3 and (Cr,Zr)2(O,N)3 films are grown in single-phase solid solution corundum-type crystal structure. The microstructure formation and phase stability will be discussed versus composition, pressure and the impact of nitrogen gas flow. It will be shown that the oxinitride materials can exhibit superior mechanical properties compared to the oxide materials.

MM 19.3 Tue 11:15 H25

Microstructure formation of magnetron sputtered Cr-V-O thin films in dependance of chemical composition — •Stefanie Spitz, Michael Stüber, Harald Leiste, and Sven Ulrich — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-AWP), 76344 Eggenstein-Leopoldshafen, Germany

The system Cr-V-O is of interest for the development of novel oxide thin films due to the ability of Cr and V to build the corundum-type structure if the oxygen supply is sufficient. Utilizing a combinatorial approach for thin film synthesis in magnetron sputtering, different Cr-V-O coatings with a wide range of compositions from Cr-rich to V-rich could be deposited in one process. An r.f. power of 500 W was applied at a segmented Cr-V target. The substrate temperature was 350 °C. The total gas pressure was kept constant at 0.4 Pa. Additionally, a substrate bias voltage up to -100 V was applied.

The elemental composition was analysed by EPMA. For thin films sputtered with 0 V bias Cr:Zr ratios of 7.4, 2.0 and 0.6 were obtained. The metal:non-metal concentration ratio shifted from 2:3 (for Cr-rich coatings) to about 2:5 (for V-rich coatings). XRD analyses indicate a nanocrystalline $(Cr,Zr)_2O_3$ solid solution in corundum-type structure for a Cr:Zr ratio of 7.4. The coatings with the highest Zr content were X-ray amorphous. Applying only a small bias voltage almost doubles the hardness values to maximum 21 GPa.