New Horizons in Coatings and Thin Films
Room Town & Country C - Session F2-1-TuM

High Entropy and Other Multi-principal-element Materials I

Moderator: Erik Lewin, Uppsala University, Sweden

8:20am **F2-1-TuM-2 Elaboration and Characterization of High Entropy Nitride Al-Ti-Zr-Ta-Hf (-N) Deposited by Reactive Magnetron Sputtering for High Temperature Applications***, **Djallel Eddine TOUAIBIA (djallel_eddine.touaibia@utt.fr)**, M. ELGARAH, S. ACHACHE,* LASMIS, France*; A. MICHAU, F. Schuster,* Commissariat à l'Energie Atomique et aux énergies alternatives (CEA) Saclay, France*; F. SANCHETTE,* University of Technology Troyes (UTT), France

AlTiTaZrHf(-N) high entropy nitrides films were deposited in various argon-nitrogen gas mixtures on glass and silicon substrates. X-ray diffraction analyses reveal a transition from amorphous to an FCC single phase by increasing the nitrogen content.

Films morphology is not influenced by nitrogen content, all films have a compact morphology. Energy dispersive spectroscopy analysis shows an increasing of the film nitrogen content when the flow rates ratio RN2=N2/Ar+N2 varies between 0 and 15% and stabilizes above. Evolution of hardness and Young's modulus are discussed and the maximum values are obtained for a flow rates ratio RN2 of 10% at 27.67 GPa and 205.56 GPa respectively. Chemical bonds and tribological performances will be discussed and high temperatures stability is investigated.

8:40am **F2-1-TuM-3 Strain-Stabilized Al-Containing High-Entropy Sublattice Nitrides***, **Andreas Kretschmer (andreas.kretschmer@tuwien.ac.at)**[1], B. Hajas,* TU Wien, Institute of Materials Science and Technology, Austria*; D. Holec,* Montanuniversitat Leoben, Austria*; K. Yalamanchili, H. Rudigier,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; M. Hans, J. Schneider,* RWTH Aachen University, Germany*; P. Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria

The impact of configurational entropy, enthalpy, and strain energy on the phase stability of high-entropy materials has not yet been investigated quantitatively. We used ab-initio calculations to predict the driving force for decomposition of 126 equimolar Al-containing high-entropy sublattice nitrides (HESN), which are all metastable with respect to all corresponding equimolar lower-entropy nitride phases. The entropy stabilization of ≈-0.06 eV/at at 1073 K is overruled by the 0.10-0.27 eV/at enthalpy-governed driving force for decomposition. Stabilization is however predicted for 22 compositions due to the -0.01 to -0.28 eV/at strain energy contribution caused by large differences in equilibrium volume between the HESN and their decomposition products. The predicted stabilities were validated with diffraction and tomography data of 9 annealed nitride systems. Hence, it is evident that only strain enables the stabilization of the here studied Al-containing HESN, while the entropic contribution is overruled by endothermic mixing.

9:00am **F2-1-TuM-4 Structural and Mechanical Properties Investigation of a New TiTaZrHfW(-N) Refractory High Entropy Films Deposited by Reactive Magnetron Sputtering***, **Abdelhakim Bouissil (abdelhakim.bouissil@utt.fr)**, S. Achache, F. Sanchette, M. El Garah,* LASMIS, Antenne de Nogent, Université de Technologie de Troyes, France

In the last decade, refractory high entropy thin films have attracted more attention due their superior proprieties at high temperatures [1]. Besides the thermal stability, these new materials present a good resistant to oxidation and can also keep good mechanical properties, high hardness and elastic modulus etc, at temperature up to 1600 °C, which is interesting compare to conventional alloys [2][3]. TiTaZrHfW(-N) films are synthesized by reactive magnetron sputtering in various argon plus nitrogen atmospheres. The microstructure, mechanical and thermal properties are investigated. Optical emission spectroscopy is performed to analyze the target nitriding conditions and to optimize the deposition parameters. The nitrogen flow rate ratio $R_{N2}=\Phi_{N2}/(\Phi_{N2}+\Phi_{Ar})$ is varied from 0 to 30%. XRD analyses show a transition from an amorphous structure to FCC single phased films once the nitrogen is added (5%). By increasing the nitrogen flow rate, preferential orientation from {111} to {200} is observed. The morphology of the films changes from compact to columnar when the nitrogen ratio exceeds 5%. The hardness and Young's modulus are also studied and the maximum values, 29 GPa and 257 GPa respectively, are obtained at R_{N2}= 9%. All nitrides show a good thermal stability under vacuum at 800 °C for three hours compared to metallic film, for which phase transition occurs.

[1] O. N. Senkov, D. B. Miracle, K. J. Chaput, et J.-P. Couzinie, « Development and exploration of refractory high entropy alloys—A review », *J Mater Res*, vol. 33, nº 19, p. 37, 2018.

[2] P.-K. Huang et J.-W. Yeh, « Inhibition of grain coarsening up to 1000°C in (AlCrNbSiTiV)N superhard coatings », *Scr. Mater.*, vol. 62, nº 2, p. 105–108, janv. 2010, doi: 10.1016/j.scriptamat.2009.09.015.

[3] O. N. Senkov, G. B. Wilks, J. M. Scott, et D. B. Miracle, « Mechanical properties of Nb25Mo25Ta25W25 and V20Nb20Mo20Ta20W20 refractory high entropy alloys », *Intermetallics*, vol. 19, nº 5, p. 698–706, mai 2011, doi: 10.1016/j.intermet.2011.01.004.

[1] **Graduate Student Award Finalist**

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