Protective and High-temperature Coatings
Room Town & Country D - Session MA4-3-WeA

High Entropy and Other Multi-principal-element Materials III

Moderators: Jean-François Pierson, IJL - Université de Lorraine, France, **Pavel Soucek**, Masaryk University, Czechia

2:00pm **MA4-3-WeA-1 Few-Layered Multi-Transition Metal Chalcogenide Heterostructured Alloy Absorber for High-Performance Photodetector***, Chia-Ying Su [neowwow1114@gmail.com],* National Cheng Kung University, Taiwan*; I-Hsi Chen, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

Few-layered MoWSSe alloy with composition spread was synthesized using salt-assisted atmospheric pressure chemical vapor deposition. A heterojunctionphotodetector device was then made by connecting two electrodes to two areas that across a composition gradient. Basic material characteristics the photodetectorperformance were examined. We demonstrate that the photodetector exhibits the highest performance under visible light among a wide range of the incident light, witha responsivity greater than 10 A/W, detectivity over 5×10 10 jones, and external quantum efficiency exceeding 3000%. Even in the near-infrared wavelength range,the device still shows a responsivity greater than 1 A/W, detectivity over 5×10 9 jones, and external quantum efficiency over 150%. The rise time was also less than 5milliseconds. The outstanding performance of this photodetector device is attributed to the multiple p-n heterojunctions formed within a few-layered composition-gradientMoWSSe alloy, generating an internal electric field that facilitates the separation of photo-generated electron-hole pairs.

2:20pm **MA4-3-WeA-2 Sputter Deposition of Ta-W-Au-Bi High Entropy Alloys for Inertial Confinement Fusion Hohlraums***, Daniel Goodelman [goodelman1@llnl.gov],* Lawrence Livermore National Laboratory, USA*; Nikhil Vishnoi, Gregory Taylor, Eunjeong Kim, Alison Engwall-Holmes, Swanee Shin, David Strozzi, Brandon Bocklund, Scott Peters, Sergei Kucheyev, Leonardus Bimo Bayu Aji,* Lawrence Livermore Laboratory, USA

The hohlraum is a centimeter-scale sphero-cylindrical cannister used as the housing for a hydrogen fuel capsule in an indirect-drive inertial confinement fusion (ICF) target. The hohlraum is a critical component in increasing the ICF energy yield. Our simulations with the radiation hydrodynamics code LASNEX suggest that the fusion yield can be improved by using hohlraums made of Ta-W-Au-Bi high entropy alloys (HEAs). However, the magnetron sputter deposition of these HEAs with low porosity and submicron grains remains a challenge. Here, we examine how tailoring the main deposition process parameters, including the average plasma discharge power, working pressure, substrate bias, target-to-substrate distance, and substrate temperature, can be leveraged to enable the fabrication of Ta-W-Au-Bi films with a dense microstructure and high electrical resistivity, thus providing a promising path forward for the development of next-generation ICF targets.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 23-ERD-005.

2:40pm **MA4-3-WeA-3 ADREnALINe : Accelerated Design of Revolutionary Entropy-Augmented, Lasting and Innovative NitridEs – First Results on Oxidation Resistance of Binary and Ternary Nitrides***, Ludovic Méreaux,* IRCER, France*; Edern Menou, Thomas Vaubois,* SAFRAN, France*; Cédric Jaoul,* IRCER, France*; **Marjorie Cavarroc [marjorie.cavarroc@safrangroup.com]**,* SAFRAN, France

Increasing aircraft engine temperature is one method, amongst others, to decarbonize aviation. But at high temperature, *e.g.*, 1200 °C, metallic materials performances are drastically decreased due to the effect of hot corrosion. To limit this impact, metallic materials need to be protected with dedicated coatings with adequate properties, which Entropy-augmented ceramics could feature.

However, the composition space of complex ceramics is very wide, and comparatively very few bibliographical data are available as these specific ceramics have not been widely studied to date. While the use of a data-driven screening tools to identify relevant compositions appears necessary, it is not sufficient as (1) it requires data to be trained on, and (2) final properties should be experimentally assessed.

Due to considered temperatures, coatings based on refractory elements such as Zirconium (Zr), Niobium (Nb), Molybdenum (Mo), Hafnium (Hf) ; Tantalum (Ta), Tungsten (W), Ruthenium (Ru) or Rhenium (Re), combined with Carbon (C), Nitrogen (N) or Boron (B), are credible potential candidates [1]. Cheaper and more abundant elements, as Iron (Fe) and Aluminium (Al), could also be considered in the mix to comply with industrial and environmental constraints.

High Entropy Alloys (HEA) (or Complex Concentrated Alloys (CCA) for their multiphase counterparts) are single-phase multielementary alloys showing original combination of properties (chemical resistance, mechanical resistance...) over a wide temperature range. The relatively new paradigm of HEA design, translated into the space of ceramics, offers new opportunities to meet high temperature requirements [2].

Two main challenges have to be overcome: achieving a single solid solution films to guarantee both material and property homogeneity throughout the coatings, and assessing the long term mechanical and environmental stability of the materials.

In this talk, we will highlight our methodology to combine numerical and experimental studies. First results about binary and ternary nitrides will be shown, together with the prospective work to come.

[1] W. G. Fahrenholtz, « A Historical Perspective on Research Related to Ultra-High Temperature Ceramics », in *Ultra-High Temperature Ceramics*, John Wiley & Sons, Ltd, 2014, p. 6–32. doi: 10.1002/9781118700853.ch2

[2] H. Xiang *et al.*, « High-entropy ceramics: Present status, challenges, and a look forward », *J. Adv. Ceram.*, vol. 10, n° 3, p. 385–441, 2021, doi: 10.1007/s40145-021-0477-y

3:00pm **MA4-3-WeA-4 Effect of Substrate Bias on Structural and Mechanical Properties of (MoNbTaW)N Coatings Deposited by Reactive DC Magnetron Sputtering***, **Saikumar Katta [saikumar.uoh@gmail.com]**,* University of Hyderabad, India

MoNbTaW is well known for its refractory high entropy properties which can maintain the same crystal structure even at very high temperatures without losing its mechanical properties. Nitrides of such (MoNbTaW)N will be a prime focus to get a hard and tough, mechanically stable high temperature withstanding coatings at room temperature.

In this study, (MoNbTaW)N hard coatings were deposited using a DC magnetron sputtering technique at a working pressure of 0.3Pa by varying substrate bias voltage from 0V to -200V. Optimized deposition parameters, including nitrogen flow and substrate temperature (400°C), were employed to produce dense and homogenous coatings on Silicon (100) substrates. X-Ray diffraction studies revealed that all the deposited films have Face Centered Cubic (FCC) crystal structure. A significant decrease in intensity ratio of principal reflection peak (111) to (200), from 2.39 to 0.84, is observed with increasing bias voltage from 0V to -200V. AFM studies indicated all the films have a fine granular morphology, with a maximum film thickness of 636nm at 0V, reducing to 550nm as the bias voltage is increased.

Topological analysis demonstrated that higher bias voltage led to smoother coatings, achieving an RMS roughness of < 2nm. XPS studies revealed that the covalency due to the increased bonding of p(N)-d(TM) with the increase in bias voltage. Nanoindentation studies confirmed a maximum hardness of 32 ± 2 GPa and a modulus of 345 ± 18 GPa at -200V bias. Additionally, the coatings displayed improved toughness, with the highest H/E value of 0.09 achieved at -200V.

3:20pm **MA4-3-WeA-5 Effect of Substrate Bias Voltage on Microstructure and Mechanical Behaviour of Equimolar VCrCoNi Alloy Thin-films Deposited via Unbalanced Magnetron Sputtering***, **Razie Hanafi [r.hanafi@unsw.edu.au]**,* UNSW, Australia*; Yujie Chen,* University of Adelaide, Australia*; Zhifeng Zhou,* City University of Hong Kong*; Zonghan Xie,* University of Adelaide, Australia*; Paul Munroe,* UNSW, Australia

Equimolar medium-entropy alloy VCrCoNi thin films were deposited on tool steel substrates by way of unbalanced magnetron sputtering, under different substrate bias voltages ranging from -20V to -120V. The deposited films were typically ~5.4 um thick. Variations in chemical composition as a function of bias voltage were observed, showing fluctuations in the concentrations of V, Ni, and Cr, while Co remained constant. These compositional variations arose from the interaction between the sputtered metal cations and the kinetic energy differences of the adatoms induced by changes in bias voltage. The thin films exhibited strong crystallographic textures and a microstructure characterized by ultrafine (< 5 nm) equiaxed grains. Changes in phase composition were also observed with variations in bias voltage. Hardness values ranged from 11 GPa to 14 GPa, peaking at -100 V bias. Additionally, scratch resistance and wear performance were examined, revealing correlations between microstructural characteristics and tribological behaviour.

3:40pm **MA4-3-WeA-6 Microstructure, Mechanical and Corrosion Properties of Reactively Sputtered (TiVCrZrNbMo)N High-Entropy Nitride Coatings***, **Žan Gostenčnik [zan.gostencnik@ijs.si]**, Aljaž Drnovšek, Matjaž Panjan, Matej Drobnič, Miha Čekada,* Jožef Stefan Institute, Slovenia

Since their discovery in 2004, high-entropy materials have been widely studied for their exceptional properties and broad application potential. Among these, high-entropy nitride coatings have emerged as promising candidates for protective coatings due to their superior mechanical and thermal properties. In particular, coatings containing refractory elements exhibit strong bonding with nitrogen, further enhancing their performance.

In this study, high-entropy nitride coatings composed of six refractory elements were synthesized with reactive direct current magnetron sputtering. The nitrogen flow ratio $R_N = N_2/(Ar + N_2)$ was varied from 0 to 50 % under a constant total gas flow to investigate the impact of nitrogen concentration on microstructure, crystal structure, mechanical properties, and corrosion resistance.

Microstructural and crystallographic analyses were conducted using X-ray diffraction (XRD), atomic force microscopy (AFM), and scanning electron microscopy (SEM). Elemental composition and chemical bonding were examined by X-ray photoelectron spectroscopy (XPS) and energy-dispersive spectroscopy (EDS). Mechanical properties were assessed using nanoindentation and profilometry, while corrosion resistance was evaluated using potentiodynamic polarization measurements.

XRD analysis revealed an amorphous structure for the coating without nitrogen, while nitride coatings exhibited a face-centered cubic (fcc) crystal structure. SEM imaging showed a columnar cross-section morphology. Hardness exceeded 30 GPa, while the reduced elastic modulus surpassed 250 GPa. Additionally, the coatings demonstrated enhanced corrosion resistance, highlighting their potential for protective applications.

4:00pm **MA4-3-WeA-7 High-Entropy Spinel Oxide Nanoparticles Achieve Record Low Thermal Conductivity and Diffusivity at High Temperatures***, **Yu Pei [y2pei@ucsd.edu]**,* University of California at San Diego, USA*; Renkun Chen, Ka Man Chuang, Sarath Adapa,* University of California San Diego, USA

Achieving efficient thermal insulation at high temperatures is critical for applications such as concentrating solar thermal (CST) and other thermal energy systems. Recent advancements in high-entropy ceramics offer a promising approach to tailoring thermal conductivity while maintaining excellent thermal stability. In this study, we demonstrate the realization of ultra-low thermal conductivity and diffusivity in ambient air using densely packed nanoparticle (NP) assemblies composed of high-entropy spinel oxides (HESOs) with more than five cation species. Unlike conventional porous thermal insulators, HESO-8 NP pellets achieve a high packing density while effectively suppressing all three major heat transfer mechanisms—solid conduction, gas conduction, and thermal radiation.

Our measurements reveal that the thermal conductivity of HESO-8 NP pellets remains as low as ~0.1 W m^{-1} K^{-1} at high temperatures, approaching the conductivity of air. This remarkable reduction in heat transport arises from three key factors: (1) suppressed solid conduction due to minimal interparticle contact, (2) reduced gas conduction via nanoscale interstitial spaces, and (3) significantly attenuated thermal radiation enabled by the infrared-absorbing metallic spinel structure. Additionally, the relatively high packing density of these pellets results in much lower thermal diffusivity than aerogels, effectively delaying heat propagation under transient heat flux conditions.

Beyond their superior thermal insulation properties, the HESO NP pellets exhibit excellent thermal stability in air at elevated temperatures. Their high-entropy spinel structure resists coarsening (sintering), ensuring long-term stability in particle size and thermal performance. These findings highlight the potential of high-entropy oxide nanostructures as next-generation thermal insulation materials for high-temperature applications.

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