

Protective and High-temperature Coatings Room Palm 3-4 - Session MA3-1-TuM

High Entropy and Other Multi-principal-element Materials I

Moderators: Frederic Sanchette, Université de Technologie de Troyes, France, Frédéric Schuster, CEA, France

8:00am **MA3-1-TuM-1 A Combinatorial Approach to Develop Sputter-Deposited Lanthanide-Containing High Entropy Alloys for ICF Applications**, **Daniel Goodelman** [goodelman1@llnl.gov], Lawrence Livermore National Laboratory, USA; **Minsuk Seo**, Lawrence Livermore National Laboratory, Republic of Korea; **Gregory Taylor**, **Alison Engwall-Holmes**, **Swanee Shin**, **David Strozzi**, **Brandon Bocklund**, **John Chesser**, **Jimmy Aut**, **Sergei Kucheyev**, **Leonardus Bimo Bayu Aji**, Lawrence Livermore National Laboratory, USA

In indirect-drive inertial confinement fusion (ICF) experiments at the National Ignition Facility (NIF), the hohlraum plays a critical role in achieving increased implosion yield, as it drives the fuel capsule's compression. Our simulations with the radiation hydrodynamics code LASNEX suggest that the fusion yield can be improved by using hohlraums made of high entropy alloys (HEAs) containing rare-earth (RE) elements. Here, we present results from a systematic study using combinatorial radio-frequency magnetron co-sputtering to develop a family of Gd-Ta-W-Au-Bi coatings with properties favorable for ICF applications, including high electrical resistivity for consideration in magnetically-assisted ICF schemes. These results provide a framework for the future development of RE-HEA hohlraum materials.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 26-ERD-011.

8:20am **MA3-1-TuM-2 Lanthanide- and Actinide-Containing High-Entropy-Alloy Coatings for Inertial Confinement Fusion Hohlräume**, **Leonardus Bimo Bayu Aji** [bayuaji1@llnl.gov], Lawrence Livermore National Laboratory, USA

A hohlraum, centimeter-scale spherocylindrical heavy-metal cans with wall thicknesses of 10–100 μm , is a key component of indirect-drive inertial confinement fusion (ICF) targets, as they determine the x-ray drive that implodes the fuel capsule. Our simulations predict that hohlraums made from rare-earth-containing high-entropy alloys (RE-HEAs) or depleted-uranium-containing high-entropy alloys (DU-HEAs) can achieve significantly higher x-ray coupling efficiencies than the best-performing single-element hohlraums made from Au or DU. Here, we present our progress in developing sputter-deposited RE- and DU-HEAs with material properties compatible with ICF target fabrication processes.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and LDRD project 26-ERD-011.

8:40am **MA3-1-TuM-3 Machine Learning Assisted Design of Complex and High Entropy Alloys by Hybrid Hipims/Pulsed Dc Pvd Process for Low Carbon Energy Applications in Extreme Environments**, **Paul Foulquier** [paul.foulquier@cea.fr], CEA-INSTN, France; **Frédéric Schuster**, **Ryma Haddad**, **Fanny Balbaud-Célérier**, CEA, France; **Jean-Philippe Poli**, CEA List, France; **Eric Monsifrot**, AZ Concept, France

INVITED

Materials and Data sciences convergence is the new paradigm governing the discovery acceleration of new materials, always more complex and integrating, in a virtuous approach, new durability and sovereignty requirements. Every great transitions are concerned: towards a sustainable future and energies, towards frugal digital applications, towards a medicine of the future always more personalised. This dynamic is organised at the national level by the PEPR DIADEM, a program gathering universities and research institutes to shape and promote this trend.

To achieve these ambitious goals of discovery acceleration, the role of acceleration platforms and self-driving laboratories is more and more significant. If numerical simulation tools are always more coupled to artificial intelligence approaches and allow the realisation of custom-made materials, in reality things are often much more complex. Indeed, no material can be made without elaboration processes and any materials keeps the memory of its elaboration process.

In this race to the discovery acceleration of materials, artificial intelligence may play a significant role in always more complex synthesis and shaping processes proficiency. Any types of Materials are concerned by these new approaches: metals, polymers, ceramics, composites including the industrials sectors in which they are involved : mobility, energy, microelectronics, construction, health. Among these high impact generic

processes for many industrial sectors, thin film deposition technologies play a key role, in particular driven towards excellence by constraints and specifications imposed by the requirements always more specific of microelectronics applications.

We will present developments for applications in extreme environments using a hybrid pulsed direct current/HiPIMS system with multiple cathodes. In particular, these developments are related to applications in nuclear reactors.

In particular, a new approach to discovering new HEA-type coatings for corrosion in molten salts for small modular reactors will be presented. We will explore the feasibility of Ni-Al-Cr-Mo alloys.

Combinatorial approaches made possible by instrumented multi-target PVD technologies, coupled to artificial intelligence allowing the extraction of inter-parametric relations between processes parameters, are at the heart of this study dedicated to the development of a hybrid pulsed-DC/HiPIMS PVD process digital twin for the deployment of complex coatings for extreme media.

9:20am **MA3-1-TuM-5 EELS Study of Fe–Co–Ni Phosphides electrocatalysts for Hydrogen Evolution Reaction**, **Chun-Te Chiang** [tony25477210@gmail.com], Southern Taiwan University of Science and Technology, Taiwan; **Yu-Min Shen**, National Dong Hwa University (NDHU), Taiwan; **Yu-Tsung Lin**, **Jow-Lay Huang**, National Cheng Kung University (NCKU), Taiwan; **Sheng-Chang Wang**, Southern Taiwan University of Science and Technology, Taiwan

Abstract

Hydrogen is widely recognized as a promising clean energy carrier, with the hydrogen evolution reaction (HER) serving as a crucial step in sustainable hydrogen production. Transition-metal phosphides have attracted considerable attention owing to their excellent electrical conductivity and catalytic activity. In this study, Fe–Co–Ni phosphides were synthesized via a solution-based precursor route followed by phosphorization, forming nanostructured multimetallic phases with uniform morphology. Transmission electron microscopy (TEM) revealed nanoscale features, while energy-dispersive X-ray spectroscopy (EDS) confirmed the homogeneous distribution of Fe, Co, and Ni.

Electron energy loss spectroscopy (EELS) played a central role in elucidating the electronic structure evolution of the catalysts. The spectra revealed distinct edges corresponding to O (538.5 eV), Fe (712.0 eV), Co (783.0 eV), and Ni (857.0 eV), clearly reflecting the hybridization between metal 3d and P 2p orbitals and providing direct evidence of charge redistribution among the transition-metal sites. These findings demonstrate the strong correlation between the local electronic configuration and catalytic performance.

Electrochemical analysis further confirmed that Fe–Co–Ni phosphides exhibit remarkable HER activity, requiring only -0.176 V overpotential to reach -10 mA cm^{-2} . The polarization (i–V) curves showed rapid current response and low activation energy, while a Tafel slope of 109 mV dec^{-1} indicated a favorable Volmer–Heyrovsky mechanism. Long-term chronoamperometric measurements verified excellent durability, and subsequent durability and accelerated cycling tests lasting up to 100 hours will be conducted to comprehensively evaluate structural and electrochemical stability under realistic conditions.

This work not only demonstrates the successful synthesis of multimetallic phosphides but also highlights EELS as a powerful tool for probing the structure–property relationship, offering valuable insights for the rational design of efficient and durable hydrogen electrocatalysts.

Keywords: NiCoFeP ; EELS; electrocatalyst

9:40am **MA3-1-TuM-6 Solid-State Synthesis and In-Situ XRD Analysis of Titanium-Based Composite Oxides for Lithium-Ion Battery Anodes and Application**, **Guan-Hong Lin** [m56144031@gs.ncku.edu.tw], **Hsing-I Hsiang**, National Cheng Kung University (NCKU), Taiwan; **Yu-Min Shen**, National Dong Hwa University (NDHU), Taiwan

The rational design of multi-component oxide systems provides an effective pathway to balance high capacity and structural robustness in lithium-ion battery anodes. In this study, $\text{TiO}_2\text{-SnO}_2$ composite solid solutions were synthesized via a controlled solid-state reaction to explore the interplay between structural evolution and electrochemical performance. Structural analyses (XRD and TEM) confirmed the partial incorporation of Sn^{4+} into the rutile TiO_2 lattice, accompanied by limited phase segregation into SnO_2 -rich domains at higher Sn contents. The coexistence of solid-solution and segregated regions generated a nanoscale heterostructure that enhanced

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Li⁺ diffusion and mitigated volume fluctuation during cycling. Among the synthesized samples, ST1450 initially delivered the highest capacity of 635.5 mAh g⁻¹ at 0.2 C, but gradually declined to 231.9 mAh g⁻¹ after 100 cycles, corresponding to the lowest degree of phase segregation. Electrochemical impedance spectroscopy (EIS) and distribution of relaxation time (DRT) analyses revealed that coherent TiO₂/SnO₂ interfaces effectively facilitated charge-transfer kinetics while preserving mechanical integrity. The optimized ST1450 sample exhibited an extremely low charge-transfer resistance of 3.85 Ω, reflecting improved electronic transport pathways. Furthermore, in-situ XRD measurements directly captured phase transitions during lithiation and delithiation, providing crucial insight into the dynamic reaction mechanism. The observed spinodal decomposition within the TiO₂-SnO₂ system forms a self-organized nanoscale microstructure that reinforces both ionic transport and structural stability. These results elucidate the lithiation pathway of TiO₂-SnO₂ composite oxides and highlight spinodal decomposition as a promising strategy for developing structurally adaptive, high-performance oxide anodes for next-generation lithium-ion batteries.

Keywords: **Composite oxides, Anode materials, Fast-charging materials, In-situ XRD, Solid-state reaction**

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