Renewable Energy and Energy Storage
Room Naupaka Salon 4 - Session RE2-TuM

Materials for Energy Conversion

Moderator: Ryan Richards, Colorado School of Mines

10:20am **RE2-TuM-8 Physical Properties Control of Metal-Hydride Thin Films and Application of Autonomous Synthesis Systems**, ***Ryota Shimizu,*** The University of Tokyo, Japan **INVITED**

Hydrogen-containing compounds have been attracting considerable attention. Until now, extensive research has focused on hydrogen energy applications such as hydrogen storage systems and fuel cells. However, recent research has diversified into various fields. For example, among various hydride materials, the ionic conductivity of Li^+ and Na^+[1] ions and hydride (H^-) ions[2] has been reported, with potential applications in electrochemical devices. Furthermore, discoveries of optoelectronic properties in rare-earth oxyhydrides[3] and high-temperature superconductivity under ultrahigh pressure[4] have opened new directions in solid-state physics and solid-state chemistry.

One unique characteristic of hydrogen is its flexible charge state. Hydrogen has an intermediate electronegativity among all elements, allowing it to exist as H^+ (proton), H (atomic), or H^- (hydride) depending on the surrounding environment. Therefore, if this charge state can be controlled by external fields, it is possible to develop devices with dramatically altered physical properties.

Our aim is to create epitaxial thin films of these intriguing metal hydrides and explore their applications in material property research and electronic devices. To date, we have successfully achieved the epitaxial growth of metal hydrides such as TiH_2, NbH, MgH_2 (hydrogen storage materials), YH_2 (smart mirrors), and EuH_2 (ferromagnetic semiconductors)[5] using reactive sputtering techniques. We have also succeeded in the epitaxial growth of yttrium oxyhydrides (YO_xH_y)[6] and calcium nitride hydrides (Ca_2NH)[7] through anion complexation with reactive gases like O_2 and N_2. We will present these deposition techniques and discuss the intriguing physical properties associated with hydride thin films involving electrons and ions.

Furthermore, aiming to accelerate the rapid discovery of such novel thin film materials, we have developed an autonomous synthesis system that integrates AI and robotics. In this talk, I will discuss future perspectives regarding a materials exploration system integrated with various measurement instruments.

References:

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11:00am **RE2-TuM-10 Non-Precious Metal Electrocatalysts for Anion Exchange Membrane Fuel Cells**, ***Jin-Song Hu,*** Institute of Chemistry Chinese Academy of Sciences, China

Under the carbon neutrality scenarios, the demand for fuel cell electric vehicles (FCEVs) is rapidly growing. According to the IEA report, the transportation section will demand more than 15,000 thousands of FCEVs by 2030. Besides continuing to improve the fuel cell performances, the fuel cells cost and FCEVs running cost come into attention. Anion exchange membrane fuel cells (AEMFCs) offer the opportunities for using non-precious metal based electrocatalysts for both anodic and cathodic reactions to reduce the fuel cell cost and relieve the concerns on the Pt scarcity.

This presentation will be focused on our recent efforts on the development of non-precious metal based electrocatalysts for alkaline oxygen reduction reaction (ORR) and the CO-tolerant electrocatalysts for hydrogen oxidation reaction (HOR). A couple of new strategies will be introduced to develop the efficient electrocatalysts, including a molecular-based cascade anchoring strategy for general mass production of high-density metal-nitrogen single-atomic catalysts, metastable rocksalt oxide mediated synthesis of high-density well-armored transition metal nanoparticle electrocatalysts, and interface assembly strategy for achieving high-density binary single-atomic catalysts with much improved active site utilization. Moreover, the binary active sites electrocatalysts will be introduced to synergistically boost the elementary reactions of the alkaline HOR. These results may provide new insights for the rational design and bottom-up synthesis of cost-effective and high-performance electrocatalysts for AEMFCs.

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[5] Zhao, L.; Zhang, Y.; Huang, L.-B.; Liu, X.-Z.; Zhang, Q.-H.; He, C.; Wu, Z.-Y.; Zhang, L.-J.; Wu, J.; Yang, W.; Gu, L.; Hu, J.-S.; Wan, L.-J. *Nat. Commun.* **2019,** *10* (1), 1278.

11:20am **RE2-TuM-11 Elucidating Early-Stage Lithium Growth and Dendrite Suppression Strategies in Lithium Metal Batteries**, ***Seung-Yong Lee,*** Hanyang University, Korea **INVITED**

Lithium metal batteries (LMBs) offer significant advantages over traditional lithium-ion batteries due to their high theoretical capacity and energy density. However, their practical application is hindered by the formation of lithium dendrites during charging, which leads to poor performance, reduced lifespan, and severe safety risks. Current research aims to understand and mitigate these challenges to unlock LMBs' full potential, but a comprehensive understanding of the fundamental mechanisms driving lithium dendrite formation remains elusive.

In this study, we employed various air-free techniques, including cryo-transmission electron microscopy (cryo-TEM), to investigate the early-stage growth behaviors of lithium metal. By enabling direct lithium deposition on copper TEM mesh grids within coin cell batteries, we examined lithium growth without additional sampling processes that could introduce artifacts and damage. Preliminary experiments showed that the stepped edges of certain TEM mesh grids served as preferential nucleation sites, guiding lithium growth within confined spaces. This finding highlights the potential of TEM mesh grids as effective 3D hosts for lithium metal anodes and underscores the need for caution in interpreting lithium growth kinetics using this method.

Further investigations using this approach revealed mechanisms behind lithium dendrite suppression with a lithium nitrate electrolyte additive. Air-free cryo-TEM experiments, including energy-dispersive X-ray spectroscopy (EDS) and electron energy loss spectroscopy (EELS), along with air-free X-ray photoelectron spectroscopy (XPS), identified the predominant phases of the solid-electrolyte interphase (SEI) formed with the electrolyte additive. These analyses indicated that an inorganic SEI layer significantly suppresses dendritic growth, transforming lithium deposition into a more spherical morphology. Additional controlled experiments confirmed the influence of the inorganic SEI layer on lithium morphology.

Our research advances battery technology by providing in-depth mechanistic insights and practical strategies to overcome the limitations of LMBs. By addressing the fundamental challenges of lithium dendrite formation, we pave the way for developing safer, high-performance energy storage solutions essential for future technological advancements.

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