

G2A : 에너지 환경 세라믹스

G2A-1 | A New Approach to Enhancing Electrolyte Stability in Protonic Ceramic Electrochemical Cells

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Reversible protonic ceramic electrochemical cells (R-PCECs) emerge as foundational components of low-temperature solid oxide electrochemical cells (SOCs) operating below 600 °C. Their primary significance lies in their low activation energy and high energy conversion efficiency, effectively overcoming the material/cost challenges associated with high-temperature operating SOCs. While doped barium cerate and barium zirconium-based compounds were utilized as electrolytes for their high conductivity, their chemical stability against CO₂ and high H₂O concentrations during PCEC operation is a concern. To counter this, diverse metal cations have been introduced into the A- or B-sites of Ba-based perovskite oxide, enhancing structural stability and proton conductivity. Leveraging the entropy-driven stabilization effect in multi-doped perovskite oxides ensures a consistent single phase under extreme temperatures and chemical environments. By adapting promising high entropy stabilization concepts to electrolytes and incorporating optimization through selective dopant incorporation and manufacturing processes, durable proton-conducting high entropy perovskite oxide electrolytes for R-PCECs were designed. This study presents recent progress in developing chemically and structurally stable high entropy perovskite oxide electrolytes for R-PCECs.

G2A-2 | 프로톤 세라믹 전기화학 전지의 Cr 피독 억제를 위한 Pr_{0.2}Ce_{0.8}O_{2-δ} 보호층 개발

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프로톤 세라믹 수전해 전지(Protonic Ceramic Electrolysis Cells: PCECs)는 비교적 낮은 온도 (≤ 600°C)에서 고효율 수소 생산과 이상적인 수전해 온도 선택으로 인해 스택장비의 비용절감에 대한 문제를 줄일 수 있다. 그러나 수소생산을 원활히 하려면 PCEC의 공기극에 스팀을 공급 시, 프로톤 전도성 전해질 (BaCe_{0.4}Zr_{0.4}Y_{0.1}Yb_{0.1}O_{3-δ})에 분리판으로부터 온 크롬(Cr₂O₃ vapor-phase)이 반응하여 전해질의 안정성에 문제를 발생시킨다. 본 연구에서는 우선, 크롬과 반응하지 않는 물질을 선정하기 위해서 실제 구동환경과 유사한 모델실험을 설계하여 Pr_{0.2}Ce_{0.8}O_{2-δ} (PCO20)을 중간층의 물질로 선정하였다. 그리고 젤라틴 기반의 용액 코팅 공정 기술에서 용액의 점성(amount of gelatin, mole concentration)과 열처리의 조건 최적화를 통해 약 100 nm

두께의 구조적으로 치밀한 중간층을 최초로 프로톤 전도성 전해층 위에 완벽하게 코팅할 수 있었다. 이렇게 개발된 박막 중간층은 PCEC의 초기 안정성 뿐만 아니라 장기 안정성에도 큰 역할을 할 것으로 기대된다.

G2A-3 | Electrodeposited Platinum on Nickel-Iron Layered Double Hydroxide as an Efficient and Durable Catalyst for Ammonia Oxidation Reaction.

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The growing demand for clean energy sources has propelled the search for sustainable hydrogen production methods. Hydrogen, as a clean energy carrier, holds significant promise, but current production methods using fossil fuels raise environmental concerns. Due to its high energy density, ammonia is emerging as an excellent hydrogen carrier, and research on ammonia oxidation catalysts for hydrogen production is important for the development of a green hydrogen society. While the oxygen evolution reaction (OER, H₂O→H₂+1/2 O₂) requires a high theoretical voltage of 1.23 V to initiate the reaction, the ammonia oxidation reaction (AOR, NH₃→3/2 H₂+1/2 N₂) has a much lower theoretical voltage of 0.06 V and is considered a more energy efficient method. Among single-metal catalysts in AOR, platinum (Pt) has shown the best catalytic performance, but it is associated with low stability due to Pt poisoning. The present study focuses on doping platinum into NiFe layered double hydroxides (NiFe LDHs) to make ammonia oxidation catalysts with high performance and stability compared to traditional Pt. The resulting NiFe LDH-supported Pt electrocatalysts exhibited enhanced stability and activity, due to the large surface area and the interaction between NiFe LDHs and Pt.

G2A-4 | Anode-supported SOFC에서 메탄 사용의 구동조건 도출 및 촉매 연구

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고체산화물 연료전지(Solid oxide fuel cells, SOFC)는 화학에너지를 전기에너지로 변환하는 고효율 장치로 기존의 화석연료 이용 방식에 비해 대기오염원 배출이 적어 유망한 에너지 기술로 주목받고 있다. SOFC는 주로 600 ~ 1000도에서 작동되며 고온 특성으로 인해 수소 외에도 천연가스, 석탄가스, 메탄올 등 다양한 연료를 사용할 수 있다. 수소는 성능면에서 우수하지만, 산소나 탄소와 결합한 형태로만 존재하기 때문에 별도의 분리 작업이 필요하며, 이로 인해 추가적인 에너지와 비용이 발생한다. 수소의 대체제로 메탄이 주목받고 있으며, 메탄은 액화천연가스(LNG)의 주요 구성 성분으로 공급량이 많고 비용이 저렴하여 SOFC에

적합한 연료이다. Ni cermet 기반으로 제작되는 연료극 지지형 (Anode-supported) SOFC는 중·저온에서 높은 출력 밀도를 가지는 장점으로 많은 연구가 진행되고 있지만, Ni cermet을 메탄 연료의 내부 개질 촉매로 사용할 경우 탄소 침적에 대한 취약성으로 인해 전극의 활성 표면적이 감소하며 셀 안정성이 크게 저하될 수 있다. 이에 본 연구에서는 스팀 메탄 개질(Steam methane reforming, SMR)과 같은 메탄 이용 방법을 고려하여 SOFC의 성능과 안정성을 유지하는 조건에 대한 연구를 진행하고 자 한다. 이 과정에서 전기화학 및 표면 분석을 통해 전극 비활성화 메커니즘을 분석하고 안정성과 성능을 고려한 최적 조건을 도출 하고자 한다. 또한 온도, 구동 전압, 연료/증기의 비(Steam to carbon ratio) 등과 같은 다양한 작동 조건 사이의 복잡한 상호작용을 이해하는데 도움이 되고자 하며 SMR 반응에 도움을 주는 촉매 적용에 대해 연구하고자 한다.

G2A-5 | Design of Dual-nanocomposite Structured Electrode for Robust Metal-Supported Solid Oxide Cells

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Solid oxide cells are efficient energy-conversion devices for reversibly generating electric power and fuels; however, robust cell structures and multifunctional electrodes must be provided to achieve high cell performance under multifuel conditions. Here, we present a precisely controlled metal-supported structure and Ni/YSZ-YSZ dual-nanocomposite catalyst. The thermal and shrinkage behaviors of the metal supports play crucial roles in determining the interconnectivity between cell components. Compared with micron-sized cermets, the dual-nanocomposite electrode with tremendous three-phase boundaries drastically improves cell performance by increasing the electrochemical activity for diverse fuel reactions. The developed cells exhibit maximum power densities of 1.1 and 1.0 W cm⁻² in fuel-cell mode and current densities of -0.61 and -0.5 A cm⁻² in electrolysis-cell mode (1.3 V) at 650 °C under H₂O/H₂ and CO₂/CO fuel systems, respectively. Our findings point to fundamental techniques for improving the structural stability and activity of cell components to operate in diverse fuel systems.

G2A-6 | Microextrusion-Based 3D Printing for Mesoscale Engineering of the Electrode-Electrolyte Interface in Anode-Supported Solid Oxide Fuel Cells

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The structural engineering of the electrode-electrolyte

interface in solid oxide fuel cells (SOFCs) on the mesoscale order (10–100 μm) is an innovative approach to increasing the volumetric power density of individual cells. Herein, the effects of the corrugated interface structure fabricated through microextrusion-based 3D printing are briefly reviewed and discussed. Next, to attain a higher aspect ratio of anode ridge structures, we propose microextrusion printing coupled with a temperature control method. An anode ink was prepared as an extrusion material and its rheological and wetting properties were evaluated at various temperatures. The viscosity of the ink is increased and its wettability to the substrate is reduced at lower temperatures, leading to improved shape retainability of an extruded ink. We then fabricated anode-supported button SOFCs by microextrusion-based 3D printing with and without temperature control and compared them in terms of their interfacial structures and power generation characteristics. Lowering the ink temperature increases the aspect ratio of anode ridge structures from 0.16 to 0.28, resulting in an increase in the interfacial enlargement ratio from 18% to 25%. Owing to this, the cell performance was remarkably enhanced; at 600 °C, the maximum power densities of mesostructurally engineered cells fabricated with and without temperature control are respectively 2.1 and 1.6 times higher than that of a flat cell.

G2A-7 | 저온에서의 전기화학 반응 속도 향상을 위한 GDC 전극의 니켈 나노입자의 역할

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Among various options for renewable energies, Solid Oxide Fuel Cell (SOFC) stands out as a promising power source due to its high energy efficiency. This SOFC's anode reaction was investigated using composite anodes consisting of nickel and gadolinium-doped ceria (GDC). For this anodes, there have been numerous researches about the anode's two active sites for H₂ oxidation reaction. The first one is the ceria-H₂ contact area known as the double-phase boundary (DPB). The second one is the nickel-ceria-H₂ contact area which is also known as the triple-phase boundary (TPB). Research findings have indicated that both DPB and TPB serve as active areas, but more researches need to be conducted to find the exact reason for their activity and the relative activity levels. Several analytical techniques, including XRD (X-ray diffraction), TEM (transmission electron microscopy), and Raman analysis, were employed to provide insights of the Ni-GDC active

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areas. Also, by incorporating the two active sites in the full cell's anode, we had results about the effect of the presence, amount, and the morphology of the nickel catalyst. The electrode which contains nickel nanoparticles had the most high performances compared to the pure and single-atom/doped nickel containing electrode. It is indicated by symmetrical & full cell test results. Our group's research result not only obtained the insights about the active areas of the Ni-GDC electrode, but we also achieved a remarkably high performance which surpasses the levels reported in previous studies.

G2A-8 | 리튬이차전지용 NCM 양극재 합성 및 평가

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Increasing demand for electric vehicles (EV) with extended driving distance requires that Li-ion batteries be of higher energy density with long cycle life. The state-of-the-art cathodes for Li-ion batteries are a family of materials derived from layered LiNiO_2 by substitution of Ni with such elements as Mn, Co, and Al, and one of the subgroups is known as Ni-rich NCM ($\text{LiNi}_x\text{Co}_y\text{Mn}_{1-x-y}\text{O}_2$, $x \geq 0.6$). Its parent material, LiNiO_2 , was investigated as a promising cathode material in the early 1990s, as it can offer higher practical capacities than the conventional LiCoO_2 at relatively lower voltages. Due to the several drawbacks of LiCoO_2 such as high cost of raw materials and its toxicity, development of Ni-rich NCM is ongoing to replace it. Among various synthetic routes, coprecipitation reaction is the most widely used method for the synthesis of Ni-rich NCM materials since it guarantees homogenous elemental distribution of transition metals and desired particle morphology with high tap density. The process using coprecipitation to synthesize Ni-rich NCM involves two steps: the formation of hydroxide particles (referred to as precursors) from the coprecipitation and calcination of the hydroxide precursor blended with a lithium source to produce the final NCM materials.

In this talk, the synthetic procedures of NCM hydroxides will briefly be introduced. The parameters affecting the particle density and morphology will also be summarized with possible relationships between reaction conditions and physical properties of NCM hydroxides to provide a guide for producing NCM materials with desired compositions and morphologies.

Keywords: Li-Ion Batteries, Ni-Rich NCM, Coprecipitation

G2A-9 | Direct Observation of Lattice-Strain-Induced Oxygen Loss in Layered Oxide Cathode without Cycling

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Oxygen loss is becoming a major concern in layered lithium transition metal oxides, which induces structural deterioration and electrochemical performance degradation. Although previous studies present numerous findings with cycled cathodes, differentiating electrical, electrochemical, and mechanical factors from simultaneous reactions is still challenging. In this work, we employed two types of single-crystalline cathode materials as a model system and then applied mechanical strain without any electrochemical treatment to investigate the correlation between structural change and oxygen release. We validated the presence of a lattice-strain-induced bond-disordered and further amorphous region by STEM and HREM images. Additional spectroscopic approaches, such as EDS and EELS, revealed a significant oxygen deficiency in those regions. DFT calculations further supported the concept by confirming the energetically beneficial oxygen vacancy formation under shear strain. This study shows that effective strain relaxation is an appropriate option to improve the structural stability of anion frameworks in layered oxide cathodes.

G2A-10 | Towards Nickel-Rich Layered Oxide Cathodes with Minimal Nanoscale Defects through Homogeneity-Driven Reactions for Long-Lifespan Li Rechargeable Batteries

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Ni-rich layered oxides show great promise as cathode materials for future lithium-ion batteries. However, their practical use has been hindered by rapid capacity loss due to chemical and mechanical factors, which are linked to atomic and nanoscale defects formed during synthesis. In this study, we investigate the atomic and nanoscale structural changes that occur during the solid-state synthesis of $\text{Li}[\text{Ni}_{0.92}\text{Co}_{0.03}\text{Mn}_{0.05}]\text{O}_2$, a promising cathode material. We employ a combination of X-ray and neutron scattering techniques, along with electron and X-ray microscopy, to delve into this complex relationship between phase transitions and microstructural changes. Our findings reveal that

atomic-scale defects, stemming from precursor decomposition, lead to the development of pores within and between grains. We quantitatively explain how these pore defects form and merge during Ni-rich layered cathode synthesis. Additionally, we propose a modified synthesis approach that promotes uniform reactions, reducing nanoscale defects and enhancing both electrochemical and microstructural stability.

G2A-11 | 실시간 전기화학 X선 분광법을 활용한 배터리 소재 내 리튬 거동의 불균일성 규명

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에너지 저장, 전기도금, 촉매 그리고 반도체 등 넓은 범위의 과학기술 분야에 활용되는 전기화학이론의 대다수는 전자의 이동만을 중심으로 발전했습니다. 그러나 리튬이온 배터리의 대표소재인 혼합전자이온전도체는 이온과 전자가 동시에 반응하여 이온의 이동이 전극에 미치는 영향을 중심으로 연구가 진행되어야 합니다. 다만, 이온과 전자가 동시에 전달되는 어려움 외에도, 아래와 같은 이유로 교환전류 연구에 대한 발전이 더딘 상황입니다. 첫째, 삽입 반응이 일어나는 수 나노미터의 계면이 두 고체전극과 전해질 상에 파묻혀 있어 분석이 어렵다는 점. 둘째, 삽입/탈리에 따른 고체 전극의 불균일한 상변이와 표면 반응성 변화로 인해, 열역학적 안정성으로 화학 반응의 운동 안정성을 추정할 수 있다는 Duhem-Jougeut 정리가 더 이상 통용되지 않는다는 점. 이에 본 연구진은 시분해능과-공간분해능을 동시에 지닌 X선 분광 현미경법을 사용하여 이온의 이동이 미치는 동역학적 영향을 실시간으로 측정 및 규명하고자 합니다. 액상부터 고상까지 다양한 전해질 환경에서 계면에서의 리튬 이온 거동을 제어하였고 이러한 상황에서 측정 플랫폼을 통해 내부의 확산 거동을 분석하였습니다. 이를 통해 고속부터 저속까지 넓은 범위의 전류 밀도 상황에서 모두 일관성 있게 설명 가능할 뿐만 아니라 limit of equilibrium에서는 열역학적으로 안정한 상태로 귀결되는 총괄적인 이온삽입 모델을 도출하였습니다.

G2A-12 | 단결정 리튬 코발트 산화물 상변화 거동에 관한 실시간 X-선 분석 연구

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LiCoO₂(LCO)는 1991년도 Sony 사에 의해 상용화가 이뤄진 후, 현재까지도 여전히 대부분의 양극 소재가 LCO의 결정구조를 기반으로 하는 층상 소재가 사용되고 있다. 층상 소재인 LCO는 CoO₂ 층과 Li 층이 번갈아 적층 되어있는 결정 구조를 가진다. LCO는 상용화된 지 꽤 시간이 흘렀으나 4.5V 이상의 고전압 영역에서 구동할 시 4.2~4.3V 구간에서 발생하는 상전이로 인해 빠른 용량감소가 발생한다는 문제가 있다. 본 연구에서는 이런 상전이 현상에 대해 좀 더 깊이 이해하기 위해 용융염 합성을 통해 입자 형상이 판상형과 구형으로 제어된 단결정 LCO를 만들어 X-선 회절 및 미세구조흡수 방법 등으로 면밀히 분석하였

다. (003) 면이 발달한 판상형 LCO는 충/방전 과정에서 생기는 격자 변형을 효율적으로 완화하지 못해 급격한 수명 열화를 보였지만, (110) 면이 발달한 구형 LCO는 우수한 수명 특성을 보여줌을 확인하였다. 추가적으로 구형 단결정 LCO에 Mg를 도핑한 샘플도 제작하여 LCO에서 Mg 도핑이 선호되는 자리도 알아보고, Mg 도핑의 효과로 상전이가 완화되는 것을 확인하였다. 본 연구에서 도출한 입자 형상, 우선 배향, Mg 도핑에 따른 LCO 단결정의 구조-물성-성능 간의 종합적인 관계는 다양한 층상 양극 소재를 사용한 고성능 LIB를 개발하는데 적용될 것으로 기대할 수 있다.

G2A-13 | Li₂OHX 고체전해질의 리튬이온전도에 대한 이해

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Lithium hydroxide halide antiperovskite Li-ion conductors are an ideal model system for the systematic investigation of the effect of grain, grain boundary and interfacial resistance on the total Li-ion conductivity. Their low melting point empowers the use of melting-solidification to prepare pellets with high relative density without additional sintering steps and with control over grain size. The tunability of the halogen anion in the dodecahedral site allows control over grain conductivity and interfacial chemistry, with minimal structural perturbation. In this study, we conduct a comprehensive investigation of Li-ion conduction on Li₂OHX_{1-x}Br_x antiperovskites with particular emphasis on correlating crystal structure, microstructure, and solid electrolyte interphase evolution in contact with metallic lithium.

G2A-15 | Stable TiO₂(B) epitaxial electrodes with high capacity for all-solid-state nanobatteries

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¹Korea Institute of Science and Technology, ²Deagu Gyeongbuk Institute of Science and Technology, ³Oak Ridge National Laboratory, ⁴University of Cambridge TiO₂(B) stand as a promising contender for a lithium-ion battery electrode material due to its unique pseudocapacitive and one-dimensional rapid ion channels. However, previous TiO₂(B) electrodes have polycrystalline nature that impedes facilitation of ion channels. In this study, we align these ion channels through the epitaxial growth of TiO₂(B) films using pulsed laser deposition. Our TiO₂(B) epitaxial electrodes exhibit an outstanding

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capacity, close to the theoretical value of 335 mA h g^{-1} and an excellent charge-discharge reproducibility in a liquid electrolyte for ≥ 200 cycles. These results surpass those of previous nanostructured $\text{TiO}_2(\text{B})$ electrodes. Furthermore, we successfully demonstrate an all-solid-state nanobattery by substituting the liquid electrolyte with a LiPON thin film electrolyte. This configuration also shows the excellent capacity and stability. These findings emphasize the remarkable potential of $\text{TiO}_2(\text{B})$ as an electrode material in all-solid-state nanobatteries for microsystem, such as implantable devices and self-powered integrated circuits.

G2A-16 | Uniform Li Deposition induced by Lithiatable Metal Oxide Layer for Stable Anode-free Batteries

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Compared with conventional lithium (Li) ion batteries, Li metal batteries with anode-free configuration can achieve the high energy density and low cost. Despite of these advantages, there are still several technical challenges to apply anode-free cells such as formation of dendritic Li which can cause the safety concern. To solve these dendritic issues, the surface modification of current collector is desirable strategy, affecting the initial nucleation and growth of Li. In this presentation, we will present the influence of lithiatable layer on the Li deposition behavior in anode-free cells. An lithiatable metal oxide (LMO) is employed as a current-collector coating material to improve the interface affinity and provide a lithiophilic property via conversion reaction of transition metal oxide. Due to these synergistic advantages, the LMO modified current collector successfully induces homogeneous Li nucleation, resulting in the excellent cycle stability in the anode-free cell.