PG8B : 전산재료과학 및 재료분석

PG8B-1 | 항공 알루미늄 합금 기계 학습 유동 응력 모델링

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AA6061 aluminum alloy is a commonly used aviation aluminum alloy in industry, which has the advantages of high specific strength, lightweight, and excellent mechanical properties. Therefore, in order to apply this type of aluminum alloy in industrial design more reasonably, it is extremely important to study its mechanical behavior based on the flow stress behavior. Here, we introduce various machine learning models to perform learning regression modeling on the high-temperature flow behavior of AA6061 aluminum alloy. Among them, the flow behavior was obtained on a thermal compression simulator at temperatures ranging from 300 to 500 ℃ and from 0.001 to 1 s^{-1}. After verification by various statistical analysis methods, we found that the multi-layer perceptron (MLP) model exhibited the best regression performance.

PG8B-2 | Understanding the electrokinetic role of ions on electricity generation in droplet-based hydrovoltaic systems

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Hydrovoltaic is emerging as a promising energy harvesting technology with the remarkable capability of generating energy through the direct interaction of water and material. The hydrovoltaic generates volt-level potentials without any external force, and its electrical performance can be enhanced by using an aqueous solution. However, it is not clear how salt ions affect or interact with the material. Herein, the theoretical model was used to provide an in-depth analysis of working principles. The model, validated with experimental results, incorporates four physics: water flow in unsaturated porous media, transportation of ions, chemical reactions, and electrostatics. It was found that the distribution of ions is key to improving the voltage output. The higher gradient of ions' concentration leads to strong potential differences, and its asymmetry of concentration is mainly governed by the water flow and concentration distribution. Additionally, we analyzed the parametric effects of substrate porosity, and relative humidity under salt solution. The results showed that the presence of salt ions makes the electrical performance highly sensitive to porosity, but less sensitive to relative humidity. Our findings improve the understanding of hydrovoltaic mechanisms and pave the way for the practical use of hydrovoltaic systems.

PG8B-3 | Finite Element Simulation of Universal Filamentary Resistive Memory with Phase-field and Fully-coupled Physics

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Resistive memory is attracting attention because of its simple structure, high operation speed, and high data storage capacity compared to commercial charge-based memory. The conducting filament of the resistive memory using metal oxide materials is commonly known as oxygen vacancies. In the electrical operation of metal oxide base resistive memory, oxygen vacancies are created when a high electric field is applied within the insulator. When oxygen vacancies accumulate in the insulator to form a conductive filament, it is defined as LRS (low resistance state), and when the conductive filament does not exist or is disconnected, it is defined as HRS (high resistance state). In other papers using finite element analysis, the initial state was a low resistance state with a predefined or ideally assumed filament structure. In this work, we present a device simulation that can show the entire switching cycle of a resistive memory. We defined the conductive filament as one of low resistance phase using finite element simulations. We have performed fully-coupled simulations of phase-field equation and electrical and thermal governing equations. We confirmed the I-V curve and the low resistance phase of the conductive filament according to the conditions of the device structure, and compared and analyzed them according to each bipolar and unipolar operation. Furthermore, it was possible to analyze a wide range of 3D device structures such as 3D vertical RRAM.

PG8B-4 | DFT simulation을 이용한 RuO_4 전구체의 area-selective ALD

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최근 전자기기의 고성능화, 소형화 추세에 따라 반도체 소자의 선폭이 10 nm 이하로 감소하였다. 이에 10 nm 이하의 선폭에서 Cu보다 비저항이 낮은 Ru, Co 등이 차세대 금속 배선 재료로 주목받고 있으며 [1] 미세한 구조를 제조할 수 있는 Atomic Layer Deposition (ALD)에 대한 의존도가 높아지고 있다. 그중에서도 Area-selective ALD는 표면의 종류에 따라 박막의 초기 성장률이 달라지는 현상을 이용한 것으로, 현재 반도체 산업의 주요 관심사이다 [2]. Minjauw 등은 패터닝된 Si/SiO_2 기판과

RuO_4 전구체를 사용하여 Area-selective ALD를 수행하였다 [3]. 본 연구는 Density Functional Theory (DFT)를 이용하여 Minjauw 등의 실험을 모사하고, 각 표면 반응 단계에서의 흡착 에너지와 활성화 에너지를 계산하였다. 또한, 더 정확한 흡착 에너지와 활성화 에너지를 계산하기 위하여 깁스 자유 에너지를 고려하였다 [4].

[1] D.-H. Choi, Korean J. Met. Mater., 56(8), 1-6 (2018). [2] G. N. Parsons and R. D. Clark, Chem. Mater., 32(12), 4920-4953 (2020). [3] M. M. Minjauw et al., Chem. Mater., 31, 1491-1499 (2019). [4] V. Wang et al., Comput. Phys. Commun., 267, 108033 (2021).

PG8B-5 | 대기비개방 Cryo FIB-SEM을 이용한 LLZTO 고체전해질 미세구조분석

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Li 계열의 전고체배터리는 대기 및 전자빔 노출에 민감하기 때문에 시편준비 및 전자현미경적 미세구조 분석을 위해서는 극복해야 할 부분이 있다. 본 발표에서는 Cu/Li/LLATO 전고체배터리 시편을 분석한 사례와 특히 고체전해질인 Li7La3Zr1.5Ta0.5O12의 미세구조, 성분분석, 결정구조 분석 사례를 공유함으로써 시편 제작과 분석과정의 인공적 결함(Artifact)에 대해 논의하고자 한다. 시편은 펨토초레이저, 기계적 연마, 이온밀링 (CP, Cross-section polisher, LN2 colling), 집속이온빔시스템 (cryo-FIB, Focused Ion Beam) 등을 이용하였으며, 냉각-주사전자현미경(Cryo SEM)을 이용하여 미세구조를 분석하였다. 장비상황에 따라 EBSD의 경우는 상온에서만 실험을 진행하였다. LLZTO는 전자빔에 매우 민감하여 상온에서 전자빔에 노출시 Li이 용출되는 것이 확인되었으며, 대기비개방 펨토초레이저-FIB-SEM EBSD를 이용한 결정구조 분석시 기쿠치패턴(Kikuchi pattern)이 매우 빠르게 없어지면서, 결정이 비정질로 상변화 되었으며, 전자빔 노출에 의한 시편 변형 자국이 형성되었다. Li 용출은 -140도 이하로 냉각함으로써 억제할 수 있었으며, EBSD 분석은 상온에서 CMOS-type 검출기를 이용하면 고속분석이 가능하기 때문에 결정구조부석데이터를 얻을 수 있는 가능성을 확인하였다. 향후 냉각홀더를 이용하여 범용 EBSD 분석 가능성을 확인할 예정입니다.

Keywords: : LLZTO, 대기비개방, Femtosecond laser, Cryo-FIB, Cryo-SEM, EDS, EBSD

PG8B-6 | Quantum Chemical Calculations of Copper Cyanide$(CuCN)_n$(n=1-10) clusters

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Copper(I) cyanide is an important reagent in organic, organometallic, and supramolecular chemistry because of both the copper center and the versatile cyanide ligand.[1] The compound is useful as a catalyst, in electroplating copper, and as a reagent in the preparation of nitriles.[2] In this study, theoretical calculations of copper cyanide$(CuCN)_n$ (n=1-10) clusters.[3,4] We calculated the copper cyanide$(CuCN)_n$ (n=1-10) clusters using density functional theory (DFT) with a 6-311++G(d,p) basis set and obtained several low minimum energy structures of each copper cyanide $(CuCN)_n$(n=1-10) clusters. Also, we further carried out the excited state calculations for the corresponding copper cyanide$(CuCN)_n$(n=1-10) clusters using time dependent-DFT (TD-DFT).

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