PG8A : 전산재료과학 및 재료분석

PG8A-1 | Grain boundary phase complexions in tellurium: a new avenue for tuning the thermoelectric transport properties.

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Elemental thermoelectric is an attractive platform for developing innovative methodologies for high- efficiency energy conversion devices. Recently, tellurium has been projected as a superior thermoelectric option but faces significant challenges in actual implementation due to carrier scattering by grain boundaries. Here, we report that As2se3 phases in the Te matrix create a heterojunction structure, resulting in increased electrical characteristics and reduced thermal conductivity. The Grain boundary phases have an amorphous lattice that differs structurally from the Te grains. As a result, we achieved a new high zT of ~1.4 over the whole temperature range. This study elucidates the several advantages of designing a heterojunction structure for independently modifying the coupled parameters, and it opens the door to the search for high-performance thermoelectric materials in Te/As2Se3-based devices.

PG8A-2 | In-situ observation of morphological evolutions of carbon nanotube fibers under various current flowing conditions

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Carbon nanotube (CNT) possesses superior mechanical and electrical properties to conventional bulk materials, so it was expected to be utilized as active materials in various prospective applications such as electronic devices [1], energy storage devices [2], and so on. However, in many cases, the properties at nanoscale were not successfully transferred into applications at bulk scale. The assembly of CNTs into CNT fibers (CNTFs) turned out to be one of the most effective ways to transfer the unique properties of CNT into macroscopic applications. Especially, wet-spun CNTFs from the CNT liquid crystalline solution with chlorosulfonic acid ($ClSO_3H$) showed excellent electrical and specific electrical conductivities reaching 1.1×10^7 S/m and 5640 $S \cdot m^2/kg$ [3], respectively. The specific electrical conductivity of CNTF is about 85 % of that of Cu, so this work at least shows a possibility for lightweight CNTFs to replace Cu-based electrical cables. However, the electrical conductivity of CNTF is far below that of Cu (5.8×10^7 S/m). Considering the electrical conductivity of individual CNT (7.7×10^7 S/m) [4], there is still room for improvement. The electrical properties of CNTF depend on not only the properties of the individual CNT, but also the organization of CNT bundles, discontinuity, misalignment, loose packing, and impurities [5,6]. Therefore, we need to investigate how internal structures of CNTF affect electrical properties of CNTF to further improve electrical properties In pursuit of this goal, we in-situ observe the morphological evolution of CNTF at nanoscale while flowing electrical current into CNTF using in-situ transmission electron microscopy (TEM). Focused ion beam (FIB) is used for placing and thinning high quality wet-spun CNTF samples on micro-electro-mechanical-system (MEMS)-based chips for in-situ electrical experiments. The detailed sample preparation method and morphological evolutions of CNTFs at various current flowing conditions will be presented in this poster.

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PG8A-3 | 자성 입자 크기에 따른 자기유변유체 거동 모델링

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자기유변유체(Magneto-Rheological Fluid, MRF)는 외부 자기장에 의해 제어되는 스마트 재료로, 용매 오일에 분산된 세라믹 자성입자가 외부 자기장이 가해지면 일정한 방향으로 정렬되어 저항력을 생성합니다. 유체와 자성입자의 변화를 통해 자기유변유체의 주요 특성인 항복응력, 점도, 안정성 등을 조절할 수 있어 토크 전달 장치, 햅틱 소자 등 다양한 시스템에서 스마트 재료로 활용할 수 있습니다. 이 연구에서는 매트랩 모델링을 사용하여 분산된 자성입자의 크기에 따른 자기유변 거동을 분석합니다.

PG8A-4 | Exploring Oxy-Halide-Based Battery Materials Via High-Throughput Screening

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Due to the growing demand for batteries in electric vehicles and portable devices, the development of safer and more energy-efficient batteries has become more crucial. All-solid-state batteries (ASSBs) have emerged as a promising solution, offering improvements over the safety and energy density issues of conventional liquid electrolyte batteries. Among the materials for ASSBs, oxides, sulfides, and halide materials families are considered promising candidates, but there are still issues to be resolved. Oxide-based ones are stable against environmental factors like air and moisture but have lower ionic conductivity. In contrast, sulfide and halide materials offer high ionic conductivity but suffer from phase or electrochemical instability. Thus, finding materials with a balance between ionic conductivity, stability, and performance is vital for developing next-generation batteries. In this direction, a few of oxyhalide materials with excellent ionic conductivity have recently reported [1] and showed great potential for this oxyhalides families. However, oxyhalide materials are rarely explored due to their complex structural factors. Thereby their synthesizable composition, electrochemical stability, and ionic conductivity are totally unknown despite the great potential of this material family for ASSBs. Here, we employ high-throughput screening to explore over 2000 oxy-halide-based battery materials including some post-transition metal and metalloid elements. By comparing to conventional sulfide/halide battery materials, such as LLZO and LGPS, we present several potential candidate materials with wide electrochemical windows. Our findings inspire the development of novel oxy-halide-based ASSB, with the anticipation of synthesizing these newly discovered materials.

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PG8A-5 | Simulation Study of the Thermally Induced Failure in Three-Dimensional Stackable Phase-Change Memory

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The scaling of phase-change memory (PCM) with three-dimensional (3D) integration helps to reduce energy consumption by decreasing reset current (Ireset) and boost data storage density. However, it also magnifies thermal disturbance (TDB), unintentional programming of adjacent cells during reset operations, causing device reliability issues. To prevent such failures and enable further downsizing, it is imperative to quantitatively evaluate the impact of TDB under specific conditions. In this article, we suggest a fully coupled simulation model not only shows the temperature change resulting from TDB, also describes the crystallization behavior of adjacent cells. By integrating electrothermal with phase-field physics, we can consider partial crystallization induced by TDB and subsequent decreases in cell resistance. This model will contribute to provide valuable insights for overcoming downsizing limitations and optimizing 3D PCM cell designs.

PG8A-6 | 3D Simulation of Solid Phase Crystallization Process in Polycrystalline Semiconductor Films using Phase Field Method.

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In this study, we simulated the solid-state crystallization process of polycrystalline Si thin films used in the channel material of 3D NAND flash memory. we developed a custom C++ code implementing the phase filed method. Through the simulation of the grain growth process, we can observe characteristics such as grain size and the evolution of grain boundaries, which impact the electrical properties of the device. By adjusting parameters related to nucleation density, size, interfacial energy, and grain growth rates, we enhanced the simulation results to better align with actual situations. We confirmed the alignment of grain sizes between practical experiments and simulation results for the

20nm film thickness. This indicates that this model has the capability and accuracy to predict microstructure evolution. Additionally, we confirmed a tendency for the grain size to increase as the film thickness increased.

PG8A-7 | Phase field simulations of strain-induced Phase Evolution in MoTe2 for HER Catalysts

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This study explores strain-induced phase transitions in layered MoTe2 as a potential avenue for affordable hydrogen evolution reaction (HER) catalysts. Using the phase-field method, we investigate the 2H to 1T' phase transition within strained MoTe2 flakes. The simulation model portrays the MoTe2 flake as a two-phase domain, where the 1T' phase resides within a 2H phase matrix. The Allen-Cahn equation, considering interfacial mobility (M) and gradient energy coefficient (γ), captures the 1T' phase's emergence under strain. Gibbs energy difference ($\triangle G$), influenced by vertical displacement, drives the transformation. Our simulations reveal the evolution of phase transition on a 100x100 grid, reflecting experimental phase ratios. This work sheds light on the potential of strain engineering to yield cost-effective HER catalysts.

PG8A-8 | Interfacial switching memristive model by modulation of Schottky barrier height using finite element method.

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Interfacial switching, Schottky barrier modulation and diffusion profile are to be considered as key characteristics of this study. Drift of oxygen vacancies occurs along the electric field and biasing leads to the concentration of oxygen vacancies fluctuating higher or lower at one electrode. Introduction of thin interfacial layer has an eminent impact in this study as this layer consists of concentration flow and the Schottky barrier height is also situated in this layer only. A two-step simulation method is adopted for developing this model system, where drift and diffusion occurs in the first step and the second step allows the measurement of current by modulating the Schottky barrier height. Our eventual goal with this study is to develop a model for the investigation of device performance in terms of materials parameters for synapse devices. Keywords- Finite element modeling, Schottky barrier modulation, Memristor, RRAM, Interfacial switching mechanism.

PG8A-9 | Investigation on the Correlation between Electronic Conduction Mechanism and Cation Antisite Defect in $CuBi_2O_4$ for Photocathodes

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$CuBi_2O_4$, a candidate material for water-reduction photocathode, has recently gained significant attention due to its suitable bandgap with p-type semiconducting characteristics. However, few experimental investigations on its major defects and electronic structure have been conducted so far. In this research, we employ atomic-scale scanning transmission electron microscopy (STEM) combined with atomic-level energy-dispersive X-ray spectroscopy (EDS) to identify a noteworthy occurrence of Bi_{Cu}-Cu_{Bi} antisite cation intermixing. Utilizing density functional theory (DFT) calculations, we demonstrate the presence of local Cu 3d polaron states and the impact of antisite cations on hole-polaron hopping between Cu. A higher degree of intermixing leads to a greater activation energy and decreased electronic conductivity. This is attributed to the hindrance of hole-polaron hopping between Cu cations. These findings highlight the significance of employing STEM-EDS analysis and DFT calculations to identify point defects and gain a comprehensive understanding of the electronic characteristics of complex oxides.

PG8A-10 | Phase-field Simulation of Thin Film Deposition and Crystallization

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Recently commercialized semiconductor devices are mostly thin films deposited on nonplanar substrates. For example, HfO2, a high-k material used in FinFETs and MBC-FET. In addition, there are channels and ONO layer in V-NAND, and capacitors in DRAM. Its deposition profile and microstructure including grain structure and surface morphology should be engineered to obtain sufficient on-current. Conformal film inside a hole is necessary. The process modeling should be preceded in order to evaluate how the deposition profile and microstructure affect device performance by TCAD or FEM.

We developed a phase-field model (PFM) code for simulating thin film growth. In this model, it consists of three phases: a substrate, a film to be deposited, and a gas. Film is divided into amorphous and crystalline, and crystalline can have various grains. Also, gas flux,

surface reaction and surface diffusion are used as parameters for the deposition process. By controlling these process parameters, different deposition results can be obtained and the conformality of the results can be checked. This makes it possible to more accurately predict the formation of the film and the microstructure of the film during thin film deposition.

In this presentation, we will demonstrate our PFM codes for thin film simulations along with some process optimization examples. The integrated model of deposition modeling and crystallization will be explained, and the direction of the model and future work topics will be explained by comparison through various examples such as the conformality and nucleation rate of the thin film deposited on the substrate.