G8 : 전산 재료 과학 및 재료 분석

G8-1 | α-Al_2O_3 내 불소 결함에 관한 이론 연구

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Al_2O_3 and its alloys with Ga_2O_3 are used as carrier confinement layers in Ga_2O_3-based devices, which are attracting a lot of attention for high-power electronics. Knowing the impact of defects and impurities on electronic properties is essential for controlling doping in these layers. Al_2O_3 is also used as a gate dielectric in GaN- and SiC-based metal-oxide-semiconductor field-effect transistors. The quality of the oxide dielectric and of its interface with the semiconductor channel is critical for device performance, since defects or impurities can act as carrier traps, cause current leakage, or scatter carriers. Using first-principles hybrid functional calculations, we focus on the role of fluorine, which can be used as a dopant in Ga_2O_3/Al_2O_3-based heterostructures, and for which some experimental evidence of its beneficial effect on device performance has been reported, but with no clear understanding of the mechanism to date. By combining with band alignment between Al_2O_3 and semiconductors, we find that F can suppress the formation of the O-vacancy related traps in the band-gap region of semiconductors.
[1] M. Choi and C. G. Van de Walle, J. Appl. Phys. 134, 064501 (2023).

G8-2 | Investigation of thermal stress effects during annealing of HfO_2 thin films using molecular dynamics simulations

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The oxides of silicon and hafnium have been serving as the major components of the thin-film semiconductor industry. Owing to the high value of dielectric constant, hafnium dioxide finds a place in Complementary Metal-Oxide Semiconductor (CMOS) and Vertical-NAND flash memory devices. Thermal stress generated during the operation of these devices may result in defect formation at the nanoscale, which may further give rise to leakage current issues. Moreover, the presence of intrinsic residual stress during the operation has found to cause the failure of thin films by cracking, delamination, buckling, etc. We employ molecular dynamics simulations using LAMMPS to investigate the effect of thermal stress during the annealing of amorphous hafnia and silica-made thin films. The amorphous structures are modeled using the Charge-Optimized Many Body (COMB) potential that facilitate variable charge by allowing charge exchange between the constituent atoms. In this study, we report the deformation/fracture behavior of the thin films at various annealing temperatures. Our study may provide insights into the thermal issues prevalent in thin films owing to the high temperature gradient during the operation and also address the ways to alleviate such undesirable deformation behavior.

G8-3 | DFT Study on Charge Transition of Oxygen Vacancies in TiO_2-based Resistive Random Access Memory

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Formation and rupture of conduction filaments (CF) by the migration of oxygen vacancies (V_Os) are the representative mechanism of resistive random access memory (ReRAM) using the TiO_2 thin films. To describe the field-driven characteristic of ReRAM, V_Os have been assumed to be positively charged (V_O^{2+}). However, in this case, the CF should be energetically unstable due to Coulomb repulsion, contrasting to the long retention time of ReRAM. Here, comprehensive DFT calculations were performed to investigate the oxidation number (ON) of V_Os constituting the CF and changes in ON during switching. Furthermore, the kinetics of the V_Os on an atomistic scale were considered. The ON of V_Os constituting the CF were revealed to be in the range of 0 ~ +1, while the ON of the V_O released from the CF immediately becomes +2. Then, the possible origins of the coexistence of eight-wise and counter-eight-wise polarity in TiO_2-based ReRAM were suggested.

G8-4 | 동결-젤 주조법으로 제작된 다공성 하이드록시아파타이트 골지지체의 변형 속도 의존 압축 거동 분석: 탄점소성 구성 모델 활용 연구

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Artificial bone scaffolds, composed of hydroxyapatite (HA) with a porosity of ≥ 64%, were fabricated using the Freeze-gel Casting method with tert-butyl alcohol (TBA) as a solvent to ensure adequate mechanical strength. The resulting HA scaffold exhibited exceptional internal connectivity due to the continuous linking of elongated columnar pores and the arrangement of

consistent pore walls. Compression tests were conducted on the HA scaffold under varying strain rates and uniaxial compression loads, with an observed maximum yield stress ranging from 2 to 3 MPa. The overall compressive behavior was categorized into elastic, plateau, and densification regions, distinguishing it from the brittle behavior of typical ceramics and resembling that of polymer materials. To describe the compressive behavior of the HA scaffold, the Frank–Brockman–Zairi constitutive model, commonly used for simulating elasto-viscoplastic material behavior, was successfully applied. Seven material parameters, integral to the constitutive equation, were proposed for the HA scaffold through a deterministic approach for material parameter identification. These models offer the potential to simulate the mechanical performance of porous ceramic scaffolds, aiding in the prediction of long-term mechanical behavior when inserted in vivo, which can be valuable for bone defect recovery.

G8-5 | Conductive-filament simulation of resistive memory behaviors for neuromorphic applications according to applied pulse voltages and initial defect by integrating phase-field models and electrothermal

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Recently, resistive random-access memory (RRAM) has been deeply researched to apply to neuromorphic computing. So far, it is hard to use the RRAM as a synapse device. Because it is one of the most important requirements for memory to reliability that can assume the uniformized performance. However, characteristics of RRAM are sensitively affected by various factors. In other words, the variability is too severe. Therefore, controlling the variability is one of the major challenges in the RRAM device research. In this work, we investigate the factors affecting the device variability in conductive filament behaviors using a multi-physics simulation that integrates the electrothermal and phase-field models. The pulse shape is the source of the variability. Furthermore, both initial defect configuration and constituent materials, to reduce the variability in the device characteristics are investigated. Thereby it is possible to systematically generalize how those factors thermotropically and electronically affect to conductive filament.

G8-6 | 고함량 세라믹 수화-분산물의 유변물성 측정으로 이용 가능한 새로운 방법에 대한 고찰

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물에 수화시킨 세라믹 분산물은 세라믹 물질의 함량에 따라 현탁액, 슬러리, 페이스트, 반죽 (suspension-slurry-paste-putty)으로 분류할 수 있다. 이들 분산체의 농도에 따른 유변물성의 측정은 학문적, 산업적 중요성 때문에 꾸준히 연구되어 왔다. 유변물성 측정 연구 결과 세라믹 함량의 낮은 경우 현탁액의 특성상 측정중에 발생하는 침강현상이 발생하고 세락믹 함량이 높은경우는 측정 중 용매의 증발과 측정기기 표면의 미끄러짐이 발생하여 측정값의 재현성이 문제가 발생하여 이를 해결하기 위한 다양한 실험 기법들이 도입되어 사용되고 있다. 특히 최근 에너지 저장소재와 정보전자 소재 분야의 전고체 배터리용 페이스트, 열전도 페이스트, 하니콤 촉매 기반물질 등 이들 세라믹 페이스트와 반죽형상은 다양하게 이용되고 있다. 전통적으로 유변물성 측정 장비는 회전형 레오미터와 모세관 레오미터가 널리 이용되고 있다. 본 발표에서는 최근 새로운 유변물성 측정장비로 이용되고 있는 스크류 레오미터를 이용하여 고함량 세라믹 반죽의 물성측정 결과에 대해 살펴보고자 한다. 압출기와 유사한 형태의 측정기로 측정물이 외부 환경과 접촉하는 부분이 없어 회전형 레오미터에서 발생하는 최외곽영역의 불안정 및 증발현상을 막을 수 있고, 모세관 레오미터에서 발생하는 Clogging 현상을 피할 수 있어 측정 전 영역에서 재연성 있는 측정값을 얻을 수 있음을 확인하였다. 시중에서 쉽게 구할 수 있는 학습용 점토 및 지점토에 대하여 전단점도를 측정하였으며, 내부 구조와의 상관관계를 확인하기 위하여 현미경 분석을 수행하였으며 각 전단속도 별로 완화시간을 측정하여 점탄성 성질을 측정하였다. 향후 전단점도와 완화시간 등 유변물성과 내부 구조의 상관관계를 규명하는 연구를 수행할 예정이다.

G8-7 | Structure and Stability of Oxygen Vacancy Aggregates in Reduced Anatase and Rutile TiO_2

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The density and arrangement of oxygen vacancies (V_Os) play an important role in tuning the physicochemical properties of TiO_2 for different technological applications, hence motivating significant interest in the characteristics of V_Os' complexes and superstructures in this material. We present results on the geometries and stabilities of V_Os' aggregates in rutile (R-TiO_2) and anatase (A-TiO_2), using density functional theory (DFT) calculations with on-site Hubbard U repulsion. We extensively explore various possible configurations to identify the most favorable geometries of divacancies and larger V_Os' complexes. We find that divacancies prefer to lie at

second-nearest-neighbor trans positions in the same TiO_6 octahedron, and ordered chains and planar aggregates of V_Os are energetically favorable over disordered noninteracting vacancies in both A- and R-TiO_2. However, the energetic gain upon V_Os' aggregation is much larger in R-TiO_2 than A-TiO_2. As a result, vacancy complexes are stable at and above typical sample preparation and annealing temperatures (~1000 K) in R-TiO_2, whereas only one-dimensional chain structures are predicted to survive at those temperatures in anatase.

G8-8 | 마찰교반처리로 만든 알루미늄/산화 그래핀 복합재의 미세구조적/기계적 변화 연구

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본 연구는 탄소질 강화재인 산화 그래핀(Graphene oxide, GO)이 단일 패스 마찰교반처리(Friction stir processing, FSP)로 만든 알루미늄 기지 복합재(Aluminum matrix composites, AMCs)의 미세구조 및 기계적 특성에 미치는 영향을 조사한다. GO 포함여부와 상관없이 FSP 후 Al 합금에서 동적 재결정에 의해 상당한 결정립 미세화가 발생했다. AMC 내에 분산된GO의 존재는 라만분광법, 2차이온질량분석법 및 투과 전자 현미경을 사용하여 확인하였다. FSP동안 GO의 존재 및 Al 기지와의 상호작용으로 AMC는 모재 및 FSP만 수행한 Al 합금보다 우수한 기계적 특성을 나타낸다. 미세경도 분포는 전체적인 교반부의 경도 증가 및 전진부에서의 최대 경도를 나타낸다.

G8-9 | Suppression of bipolar conduction via band gap engineering for enhanced thermoelectric performance of InTe.

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InTe has recently attracted attention as a candidate for thermoelectric material due to its low thermal conductivity originating from the anharmonic bonding of In^{1+} which scatters phonons in the lattice. However, with a very narrow band gap of about 0.12eV, InTe exhibits bipolar conductivity at high temperature making it unfavorable for high temperature applications. The substitutional doping of Bi and Sb into In site is able to distort the crystal structure thereby increasing the band gap. Density functional theory calculations validates the effect of structure distortion on the bandgap. Bipolar conductivity is thus suppressed resulting in simultaneous enhancement in Seebeck coefficient and reduced lattice thermal conductivity at high temperature. An ultra-low lattice thermal conductivity of 0.27W/mK at 773K is achieved with a maximum zT of 0.75 and 0.82 for $In_{0.99}Bi_{0.01}Te$ and $In_{0.99}Sb_{0.01}Te$ respectively.

G8-10 | Green Synthesis of Lone-Pair-Driven, Brightly Emitting Lead-Free Inorganic Luminescent Member

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Zero dimensional (0D) $5s^2$-metal halide (MH) materials receive special attention for applications is solid-state lighting, optical thermography, and scintillation. However, most of the highly luminescent materials are persists with the problems of instabilities of the organic components against moisture and thermal stress, which impedes their practical usage in advanced applications. Hence, it requires highly luminescent and stable inorganic luminescent material that has not yet found. Herein, for the first time, we reported a new 0D fully inorganic luminescent member of K_2SbCl_5 exhibits a high photoluminescence quantum yield (PLQY) of 80%, which is the highest among the reported inorganic Sb^{3+}-based MHs. In addition, K_2SbCl_5 also shows a superior PL stability than hybrid MH of $(TTA)_2SbCl_5$ after exposing the samples in ambient conditions for 50 days. To understand the emission mechanism in K_2SbCl_5, we performed triplet spin state calculations and it reveals $[SbCl_5]^{2-}$ square pyramidal are only optically active emission center. Furthermore, we also fabricated the white light emitting device using K_2SbCl_5, delivers a high color rendering index and high luminous efficacy values of 94 and 118.1 lm/W, respectively. Therefore, we present the isolated $[SbCl_5]^{2-}$square pyramidal environment as a design principle for exploring highly efficient new inorganic Sb^{3+}-based luminescent members for future optoelectronic applications.

G8-11 | Development of new technology to calculate and classify complex non-metallic inclusions in steelmaking process

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Recently, as the global industrial trend has entered a new phase such as carbon neutrality and hydrogen energy conversion, interest in developing new high-performance, high-alloy steel types continues to increase. Simultaneously, despite the low quality and

diversification of raw materials, demand for the production of high-quality steel products is also increasing. In the steelmaking process, a major issue is not only controlling the composition of molten steel, but also controlling non-metallic inclusions, which are the main cause of defects in the final product. These non-metallic inclusions are reported to be produced in various morphologies and compositions depending on the alloy design and control process. In particular, in secondary steelmaking process, oxide inclusions such as Al_2O_3, $MgAl_2O_4$, and $CaO-Al_2O_3$ systems are mainly generated after de-oxidation process, and these inclusions could be analyzed using the quantity, size, image, and aspect ratio of the inclusions within a designated area using the automated scanning module of a scanning electron microscope (SEM). However, this is a technique for observing inclusions in samples quenched to room temperature, and there are limitations in identifying the state of inclusions under actual process conditions above 1773 K. Moreover, it cannot be distinguished from precipitated inclusions generated during solidification. Therefore, in the present study, to determine the level of inclusions under actual process conditions and control, we attempted to quantitatively evaluate the equilibrium phase of inclusions in molten steel using the macro function of FactSage, thermodynamic simulation software. In addition, we would like to use these results to develop a cleanliness evaluation index for the molten steel by establishing standards for classifying complex inclusion phases.