

# 第300回応用セラミックス研究所講演会

## 300<sup>th</sup> MSL Lecture

**Date/Time:** 15:00-16:00, Friday, October 16<sup>th</sup>

**Venue:** 1F Meeting Room, Building R3

**Speaker:** Dr. Minseok Choi

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**Title:** Understanding of strain and defects in complex oxides

### Abstract:

Strain-mediated control of materials properties has been extensively studied, as strain is a simple and predictive parameter for property control. In complex oxides, drastic changes in chemical and physical properties of the oxides are observed with an introduction of strains by lattice distortion or lattice mismatch. Based on first-principles calculations, we have investigated strain, defects and their interaction in prototypical complex oxides. In this talk, the role of strain and defects in the structural and electrical properties of oxides will be presented and discussed. We demonstrate that strain triggers the formation of oxygen vacancies in complex oxides by examining the tilt boundary of SrTiO<sub>3</sub> bicrystals [1]. Our calculations predict that strains lower the formation energy of oxygen vacancies, thereby enhancing the vacancy formation. Oxygen vacancies are observed in the strain-imposed regions between dislocation cores via transmission electron microscopy and electron energy loss spectroscopy. We also find that strain induced by chemical doping such as hydrogenation strongly impacts on structural and electrical properties of VO<sub>2</sub> [2]. In experiment, we observe that the massive hydrogenation process leads to peculiar phase transition of vanadium oxyhydride (H<sub>x</sub>VO<sub>2</sub>), and our calculations show that the phase transition is originated from the heavily doped electrons with cooperative interaction of huge lattice expansion.

[1] S.-Y. Choi, S. D. Kim, M. Choi *et al.*, Nano Lett. **15**, 4129 (2015).

[2] H. Yoon, M. Choi *et al.*, Under Review

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