東京大学大学院工学系研究科　総合研究機構

結晶界面工学研究室

Crystal Interface Laboratory, The University of Tokyo

Crystal Interface Lab. Seminar Series

“Materials under the microscope: From defects to functionality”

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Key to understanding material’s functionality is accurate identification of different defect configurations and concentrations. A new feature extraction scheme has been developed based on a Zernike polynomial method. Rather than just mapping atom position and intensity, it classifies local symmetry and can therefore recognize atoms at edges and boundaries as different from those elsewhere. It also shows very high noise rejection ability and represents a new promising means to link defect content to properties.

At an appropriate beam energy, it is possible to selectively sputter light atoms leaving heavier metals atoms intact. In this way we fabricated suspended monolayer Mo membranes from monolayer $MoSe_2$ films. The nucleation and subsequent growth of the Mo membranes are triggered by the formation and aggregation of Se vacancies, as seen by atomic resolution sequential STEM imaging. Various novel structural defects and intriguing self-healing characteristics are unveiled. Suspended monolayer metal membranes have never been prepared by conventional growth methods and it is likely that other metal membranes can be fabricated in a similar manner.

Single atom sensitivity is also important for developing thermoelectric materials. Whereas nanostructuring has been well appreciated, recently the key role of interstitials and interstitial clusters on thermal and electrical transport properties has also been elucidated. In piezoelectrics, gradual atomic-scale polarization rotation among co-existing phases has been recently found in lead-free piezoelectrics, a feature that seems common to all high-performance piezoelectric systems at phase boundaries. For single atom catalysis, Z-contrast imaging, electron energy loss spectroscopy combined with density functional theory is an excellent combination to unravel the origin of the catalytic activity. Also, their use as the air cathode in a solid-state Zn−air battery, has achieved good cycling stability (2500 min, 125 cycles) and a high open circuit potential (1.411 V).

Recent developments in optical sectioning will also be presented, including identification of buried extended defects and impurity segregation. A new GPU-based image simulation package for full frozen phonon simulations of focal series of millions of atoms will be described.

Main meeting room at Institute of Engineering Innovation

工学部総合研究機構９号館１階　大会議室

2019, July 9th (Tue)　15:30～17:00