Tochigi LAB.

[Microstructure & Mechanical Behavior]

Department of Fundamental Engineering

Nanoscale Strength of Materials

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https://sites.google.com/g.ecc.u-tokyo.ac.jp/nanoscale-strength

Development of atomic-resolution in situ TEM mechanical experiment system

Deformation and fracture of crystalline materials are originated from atomic displacements and atomic bond breaking. Transmission electron microscopy (TEM) is known to be one of superior techniques to directly observe the microstructures and atomic structures of matter. In situ TEM mechanical testing provides information on microstructural evolution and mechanical responses during deformation and fracture behavior. We are developing loading devices for in situ TEM mechanical testing based on MEMS technology and conducting applied in situ TEM experiments.

Fig. 1 shows a loading device for in situ TEM, atomic-resolution scanning TEM image under loading (sample: SrTiO3), and a strain map derived from the experimental image. These results indicate that our in situ experimental system has good stability to obtain fine atomic-resolution images under loading. In addition, the strain map shows a strong tensile strain is generated by stress concentration at the notch.

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- E. Tochigi, T. Sato, N. Shibata, H. Fujita, Y. Ikuhara, *Microsc. Microanal.* **25**, S2, 770 (2019).
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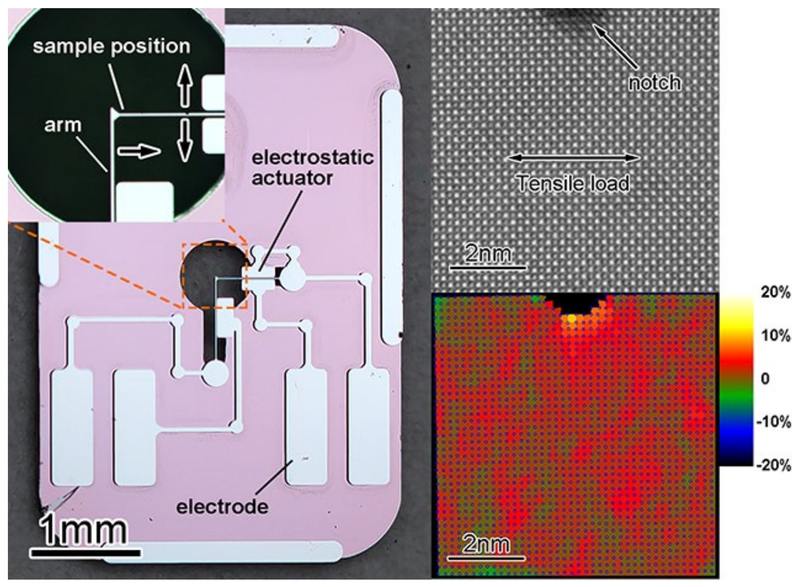

Fig. 1. Loading device fabricated by MEMS processes and atomic-resolution TEM tensile experiment of $SrTiO_3$ single crystal.

Atomistic mechanisms and dynamic behavior of deformation twinning

Deformation twinning is one of representative deformation modes of crystalline materials and forms a deformed region with mirror or two-fold symmetry within the matrix. However, little is known about detailed mechanisms of deformation twinning despite many years of study. We are conducting research on mechanisms of deformation twinning by using in situ TEM mechanical testing, atomic-resolution TEM observations, and first-principles calculations.

Fig. 2 shows a TEM image of a twin taken during in situ TEM nanoindentation (sample: α-Al_2O_3), an atomic-resolution scanning TEM image of a step structure on the matrix/twin interface, and results of atomic simulation based on first-principles molecular dynamics calculations. It was found that the growth of the rhombohedral twin is mediated by a glide motion of the step structure on the interface. Furthermore, the glide motion of the step structure is originated from coordinate motions (shuffling motions) of a five-atom group consisting of two Al atoms and three O atoms. To reveal such fundamental mechanisms of deformation phenomena expands our knowledge about a simple question: how does matter deform?

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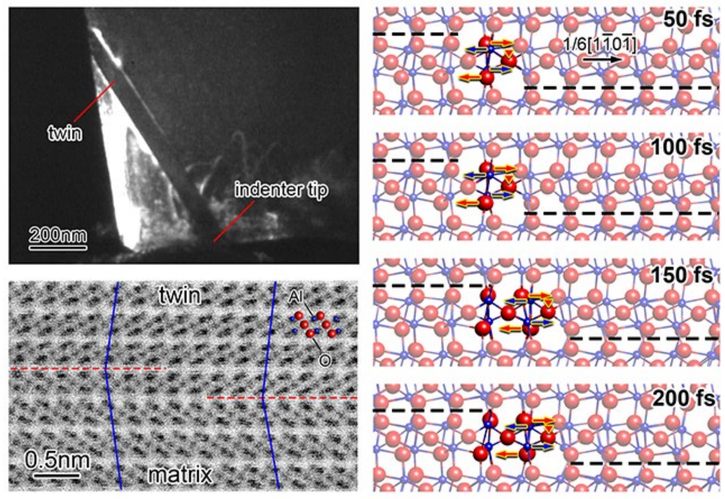

Fig. 2. In situ observations of twin in α-Al_2O_3, interface atomic structure, and molecular dynamics simulation.

Structural analysis of lattice defects

Crystals involve defect structures such as dislocations, twins, or grain boundaries, and they control materials' properties. We focus on their structural features and conduct various analytical research.

Fig. 3 shows TEM images of screw dislocation network in a low-angle twist grain boundary ofα-Al_2O_3, the core structure of the basal dislocation in α-Al_2O_3, and the basal stacking fault in 4H-SiC. These experimental data are fundamental information for firm structure-model construction and theoretical simulation. The combination of the experimental and theoretical analysis deepens our understanding about deformation mechanisms of mater, mechanical behavior, and local properties.

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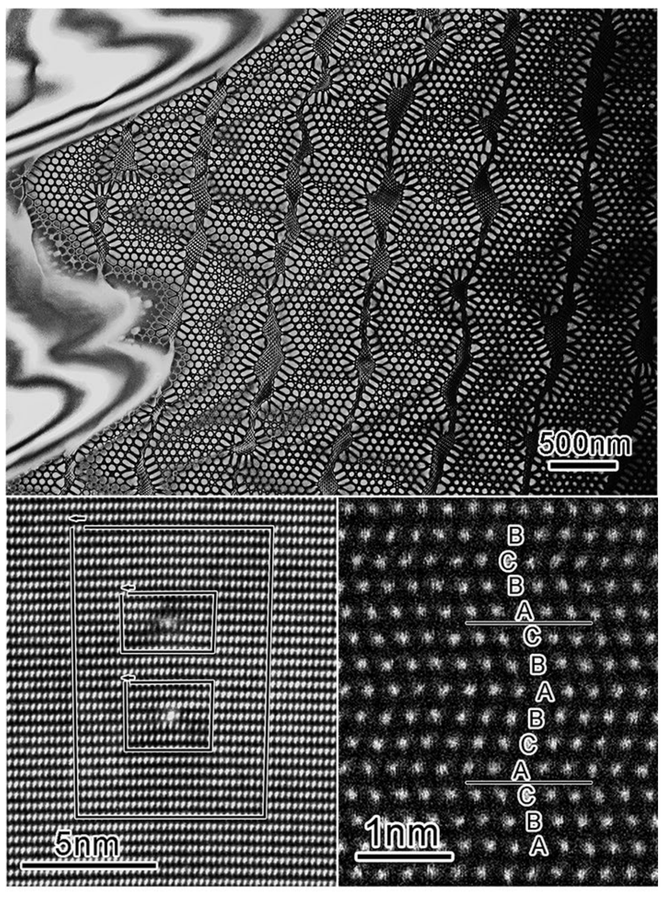

Fig. 3. Screw dislocation network (α-Al_2O_3), dislocation core structure (α-Al_2O_3), stacking fault (4H-SiC)