

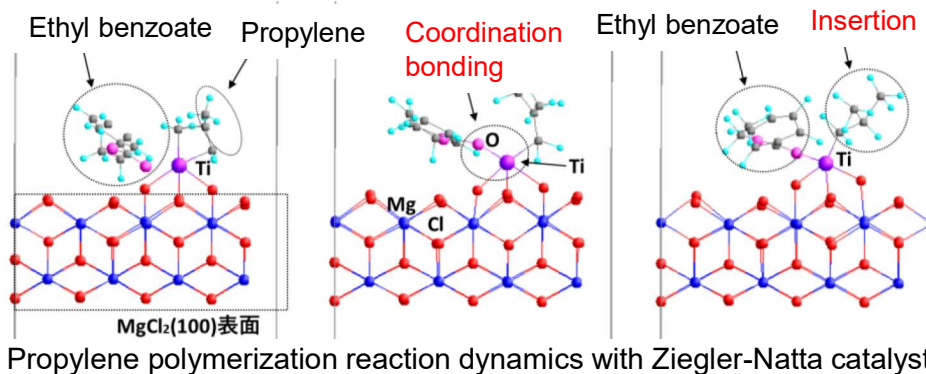
## Achievement of a safe and secure society through the control of material functions and degradation

**【Research Policy】** We will elucidate the mechanisms of function and performance of materials through atomic-level simulations and experiments, and develop molecular design, manufacturing, and evaluation techniques to prevent degradation and damage of materials used in harsh environments.

## Research Topics

# Functional Design of Materials by Atomic-Level Simulation

## ➤ Chemical Reaction Simulation of Resin Material Synthesis Process

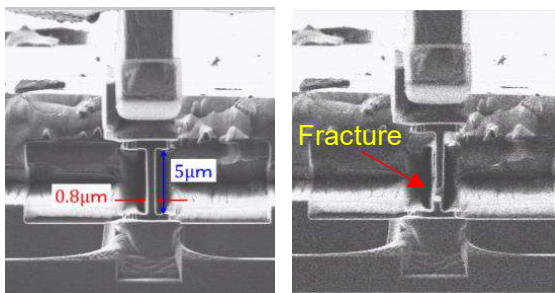


## Prediction of resin amorphous structures and properties by polymerization reaction simulations

## Development of high performance resin materials by synthesis process control

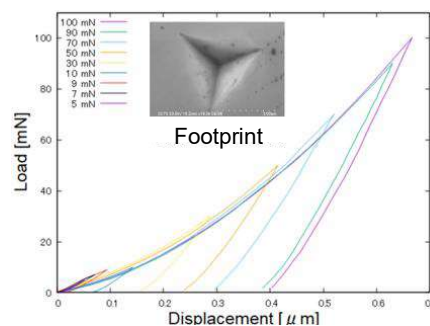
## Elucidation of Degradation and Damage Mechanisms

- Evaluation of deformation characteristics of next-generation power device materials

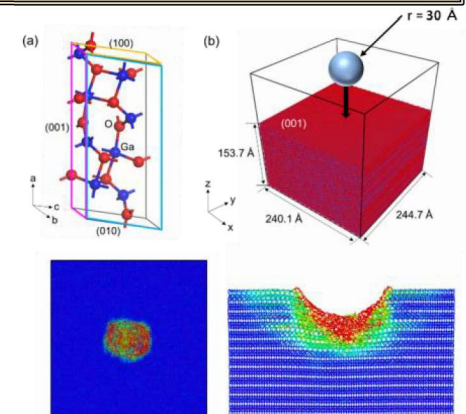


Before test

At fracture



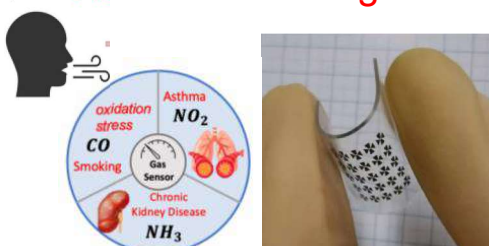
## Indentation test of Ga<sub>2</sub>O<sub>3</sub>



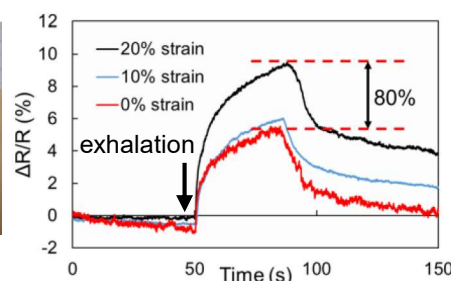
### MD simulation of the indent formation process

## Development of Carbon Material Based Health Monitoring Devices

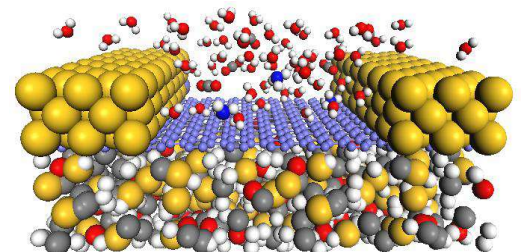
➤ Health monitoring devices applying strain-controlled two-dimensional materials



Flexible gas sensor



# Graphene-base gas detection sensor for exhaled breath



### Atomic-level simulation of graphene-based gas sensor structure