

## Research topics for graduate students for 2024

### Professor Satoshi Izumi

Department of Mechanical Engineering

Acceptable course(s)

- Master's Degree
- Doctoral Degree



#### Research Topics

Izumi group has been working on material mechanics problems and the strength and reliability evaluations by multi-scale and multi-physics simulations, in collaboration with companies and research institutes. Present research covers various fields such as semiconductor, railway, electronics, aerospace.

#### 1. Molecular dynamics simulation of SiC oxidation process [1]

Silicon carbide (SiC) is an attractive semiconductor material for applications in power electronic devices. However, the atomistic mechanism of the thermal oxidation of SiC remains to be solved. In this paper, a new Si-C-O interatomic potential was developed to reproduce the kinetics of the thermal oxidation of SiC. Using this newly developed potential, large-scale SiC oxidation simulations at various temperature were performed. The results showed that the activation energy of the Si-face is much larger than that of the C-face. Our new insight at atomistic level would contribute the fabrication process of power device.

#### 2. Reaction pathway analysis for BPD-TED conversion in 4H-SiC [2][3]

4H-SiC has been widely used as a next-generation power-device material. It is known that basal plane dislocations (BPDs) are problematic since they degrade the performance of the devices. Most BPDs are converted into harmless threading edge dislocations (TEDs) by using a step-controlled epitaxy. However, the mechanism underlying BPD-TED conversion is still not clear since this conversion occurs in the vicinity of the surface. Therefore, the purpose of this study is to elucidate the mechanism using molecular dynamics.

#### Articles Related to Research Topics

- [1] So Takamoto, Takahiro Yamasaki, Takahisa Ohno, Chioko Kaneta, Asuka Hatano, and Satoshi Izumi, "Elucidation of the atomic-scale mechanism of the anisotropic oxidation rate of 4H-SiC between the (0001) Si-face and (000-1) C-face by using a new Si-O-C interatomic potential", *Journal of Applied Physics* 123, 185303 (2018).
- [2] Yohei Tamura, Hiroki Sakakima, So Takamoto, Asuka Hatano, Satoshi Izumi, "Reaction pathway analysis for the conversion of perfect screw basal plane dislocation to threading edge dislocation in 4H-SiC", *Jpn. J. Appl. Phys.* 58 081005 (2019)
- [3] Atsuo Hirano, Hiroki Sakakima, Asuka Hatano, Satoshi Izumi, "Reaction pathway analysis for the contraction of 4H-SiC partial-dislocations pair in the vicinity of surface", *Jpn. J. Appl. Phys.* 60 085502 (2021)

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