Research topics for graduate students for 2024

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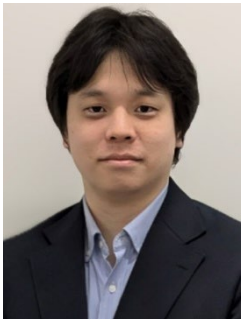

Department of Mechanical Engineering

Acceptable course(s)

- Master's Degree
- Doctoral Degree

Research Topics

We perform multiscale simulations, including first-principles analysis, molecular dynamics, and finite element analysis, to elucidate the mechanics and of materials and related phenomena. These methods also include machine learning techniques. Our current focus is primarily on, but not limited to, semiconductors and related materials.

1. Mechanical strength and reliability in SiC and other semiconductor devices [1]

Silicon Carbide (SiC) is an attractive semiconductor material for power device applications. However, defects in crystals and interfaces can significantly degrade the performance and reliability of SiC power devices. To elucidate and gain atomistic insight into the dynamics of these defects, we have performed simulations at a wide range of scales, including first-principles analysis, molecular dynamics, and finite element analysis.

2.Application of machine learning techniques to molecular dynamics simulations [2]

In recent years, the incorporation of machine learning techniques into molecular dynamics simulations has been one of the emerging research areas. In particular, the development and application of machine learning type interatomic potentials is attractive. We perform molecular dynamics simulations with universal interatomic potentials for multi-component systems. At the same time, we are developing systems to generate interatomic potentials that are applicable to practical simulations.

3. Effects of excess carriers on the mechanical properties of semiconductor materials [3]

The mechanical response of semiconductor materials to injected excess carriers is important for understanding the mechanics of materials under the operating conditions of semiconductor devices. We have studied the effects of excess carriers on the stacking fault energies and the ideal strength of crystals using first-principles calculations.

Articles Related to Research Topics

[1] H. Sakakima et al., Modeling the effect of mechanical stress on bipolar degradation in 4H-SiC power devices, *J. Appl. Phys.* **128**, 025701 (2020).

[2] H. Sakakima et al., Exploration of the mechanical properties of carbon-incorporated amorphous silica using a universal neural network potential, *J. Appl. Phys.* **135**, 085104 (2024).

[3] H. Sakakima and S. Izumi, First-principles investigation of the effects of excess carriers on the polytype stability and stacking fault energies of SiC, *J. Appl. Phys.* **134**, 155103 (2023).

Lab. Web page: https://www.fml.t.u-tokyo.ac.jp/