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[Computational Materials Science for Highly Efficient Energy Utilization]

Collaborative Research Center for Energy Engineering

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Computational Materials Science for Energy Engineering

Department of Mechanical Engineering

Computational Materials Science Approach toward Energy Materials

Utilizing various kinds of computational materials science techniques which are capable of treating from microscopic to macroscopic scale, we are trying to clarify and predict the microstructure or defect kinetics of materials in next generation energy system like solid oxide fuel cell (SOFC). In addition, we are developing completely new atomistic technologies which can overcome a time and spatial scale issues. These methodologies provides a great insight on the kinetic properties of materials from atomistic level.

- ◆Microstructural evolution of SOFC anode using kinetic Monte Carlo approach
- ◆Atomistic level simulations for cation diffusion in SOFC materials
- ◆Activation free energy computations for dislocation nucleation using accelerated molecular dynamics approach
- ◆Interfacial delamination modeling using atomistic-continuum coupling approach

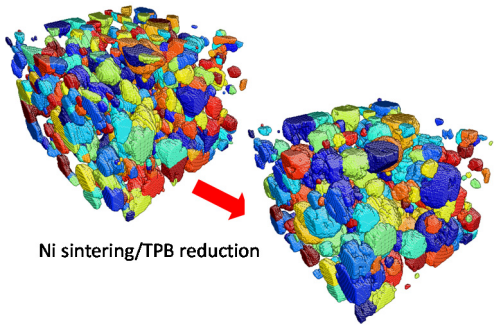


Fig1. Ni coarsening modeling during SOFC operation

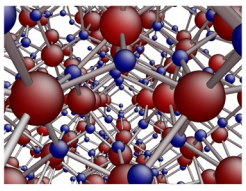
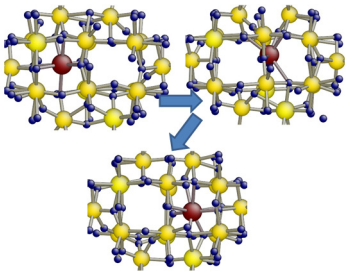


Fig2. Cation vacancy migration in YSZ electrolyte



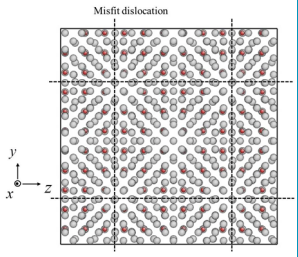


Fig3. Ni/NiO interface modeling

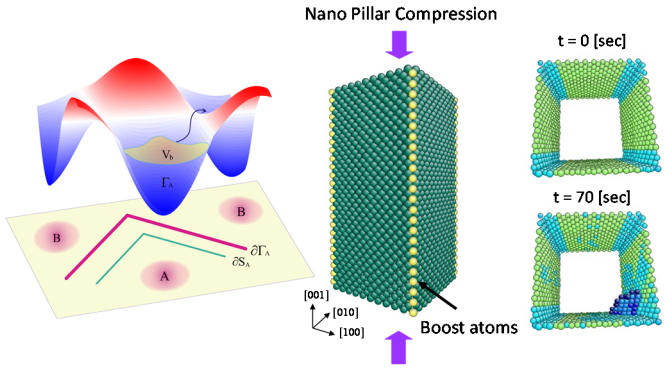


Fig4. Boost MD simulations for dislocation nucleation

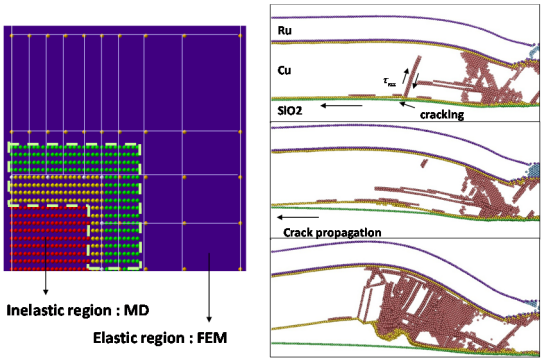


Fig5. Delamination modeling using MD-FEM coupling approach