

Simulation Technology towards the Hydrogen Use World

organized by

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While various new energies are considered instead of fossil fuel, hydrogen is attracting the most interest as a leading energy in this century. It is greatly expanding the possibility from use as a current industrial gas to the basic energy of a social system. It will be used as fuel of a fuel cell for which development is performed actively. A fuel cell immediately changes the chemical energy of hydrogen and oxygen to electrical energy. This conversion has high efficiency and low emissions. In the demand for the zero emission and the CO₂ reduction, the expectation for clean hydrogen is growing more and more.

Many scientists are studying characteristic features of hydrogen. But it is difficult to experiment the hydrogen dispersion in case of hydrogen leaks, because hydrogen has a high diffusion coefficient and low kinematic viscosity. Hence clarifying the hydrogen dispersion with numerical analysis becomes important. Furthermore, the mechanism of hydrogen embrittlement is still not clear despite many years of intensive investigation. Over the years a number of theories have been developed. Then, for example, in order to model the effects of the hydrostatic stress and hydrogen trapping due to plasticity on the hydrogen distribution in a body, a coupled diffusion elastic_plastic stress analysis is necessary. The finite element method (FEM) is a very useful tool for this purpose.

In this minisymposium, the above related numerical topics are widely accepted from macroscopic analysis using FEM to microscopic analysis using the molecular dynamics (MD) and so on.