Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Phase-field modeling of coupled dynamics of dislocation and hydrogen density fields in BCC iron based on first principles calculation[1]

HIDEKI MORI, HAJIME KIMIZUKA, SHIGENOBU OGATA, Department of Mechanical Science and Bioengineering, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka, Japan — We construct a numerical model of the coupled evolution of hydrogen-concentration and defect fields in iron based on a phase-field (PF) microelasticity theory, with coupling of the long-range elastic interactions and short-range chemical interactions that control hydrogen and dislocation motion. To obtain the physical parameters included in the PF free-energy functional, the interaction energy between a hydrogen atom and dislocation core, the hydrogen-concentration dependence of misfit energy and eigenstrains are quantitatively determined using density-functional-theory (DFT) calculations. Based on these data, we investigate a time evolution of the hydrogen-dislocation interactions under applied external stress. For atomic interaction between hydrogen and dislocation core, it is observed that hydrogen concentration distribution is affected by the motion of dislocation.

[1]Fundamental Studies on Technologies for Steel Materials with Enhanced Strength and Functions Consortium of JRCM (The Japan Research and Development Center for Metals)

Hideki Mori
Department of Mechanical Science and Bioengineering, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka, Japan

Date submitted: 01 Dec 2009 Electronic form version 1.4