Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Ab-initio and thermodynamic description of interaction of hydrogen with vacancies in fcc iron ROMAN NAZAROV, TILMANN HICKEL, JOERG NEUGEBAUER, Max-Planck-Institut für Eisenforschung GmbH — Several mechanisms of hydrogen embrittlement are associated with a significant increase of the vacancy concentration in a H-rich atmosphere. These superabundant vacancies can form vacancies clusters or even microvoids in regions of high stress (for example crack tips), facilitate the formation of brittle phases and reduce elastic properties of crystalline structure. In order to reveal the physics of this phenomenon we have employed density-functional theory (DFT) together with thermodynamic concepts. Our systematic comparison of isolated and hydrogen loaded vacancies in fcc iron with various magnetic configurations reveals that hydrogen reduces the formation energy of a vacancy. This decrease can be significant, as up to 6 hydrogen atoms can be incorporated into a vacancy. Based on our ab-initio results we developed a thermodynamic model which determines the concentrations of vacancies, of hydrogen in different interstitial positions and of vacancy-hydrogen complexes as a function of pressure, temperature and external hydrogen chemical potential. Applying this model we find dramatically increased vacancy concentrations and total hydrogen concentration in fcc iron if the material is exposed to a H-rich atmosphere.

Roman Nazarov
Max-Planck-Institut für Eisenforschung GmbH

Date submitted: 18 Dec 2009 Electronic form version 1.4