8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

Effect of Hydrogen on (110)[111] Edge Dislocation Mobility in Alpha Iron

***S.Taketomi[1], R. Matsumoto[2] and N. Miyazaki[3]**

[1] Department of Mechanical Engineering and Science, Graduate School of Engineering, Kyoto University, 606-8501
taketomi@solid.me.kyoto-u.ac.jp
http://solid.me.kyoto-u.ac.jp/

[2] Department of Mechanical Engineering and Science, Graduate School of Engineering, Kyoto University, 606-8501
matsumoto@solid.me.kyoto-u.ac.jp
http://solid.me.kyoto-u.ac.jp/

[3] Department of Mechanical Engineering and Science, Graduate School of Engineering, Kyoto University, 606-8501
miyazaki@solid.me.kyoto-u.ac.jp
http://solid.me.kyoto-u.ac.jp/

Key Words: *Hydrogen Embrittlement, Nudged Elastic Band Method, Alpha Iron, Edge Dislocation.*

ABSTRACT

Clean and new energies are expected due to environmental safeguards and energy problems. Hydrogen is one of the candidate energy sources for clean energy systems, therefore many researches and developments have been conducted. In order to realize the hydrogen energy society, the investigation into details of the hydrogen property and hydrogen effects on the environment is important. For example, hydrogen easily penetrates into metals and results in a drastic change of mechanical properties of them. It is well known as a hydrogen embrittlement. On the other hand, metal is the best material for hydrogen storage components from the economical point of view. Concerning the hydrogen embrittlement, many fracture mechanisms have been proposed. However, the hydrogen embrittlement fracture is considered to be a result of multiple phenomena. Thus the whole fracture mechanisms of hydrogen related fracture have not yet been clarified. One of the remarkable effects of hydrogen on the material property is an enhancement of the plasticity localization, and it is called HELP (Hydrogen Enhanced Localized Plasticity). I.M.Robertson et al.[1] conducted *In-situ* observation of the separation distance of dislocations under hydrogen gaseous environment using Transmission Electron Microscope (TEM) and revealed the reduction of the distance between dislocations. Such a plasticity localization is observed in a large number of materials and slip systems[2]. Therefore, this experimental result is considered to be a powerful evidence of HELP. This experimental observation, however just shows the reduction of the separation distance of dislocations under hydrogen gaseous environment. The exact reason for this reaction is unclear (e.g. reduction of the interaction force between dislocations, reduction of the energy barrier for dislocation motion or the external force due to gaseous pressure). According to the elastic analysis conducted by P.Sofronis[3], reduction of the separation distance is caused by the

reduction of the interaction force between dislocations. However, the hydrogen concentration at the dislocation core in the analysis is extreamly high, and could not take into account the effect of dislocation core due to the limitation of the theory of elasticity. On the other hand, *ab initio* study showed the reduction of pierls potential for aluminum in the presence of hydrogen. Moreover, we investigated the reduction of energy barrier for (112)[111] edge dislocation motion in alpha iron in the presence of hydrogen[4]. However, bcc structured alpha iron have the (112) and (110) slip systems in nature. Therefore in this study, analyses are conducted based upon atomic models of alpha iron including the effect of dislocation core structure to investigate the effect of hydrogen on the mobility of dislocation. The estimation of energy barrier for dislocation motion is conducted based on the Nudged Elastic Band (NEB) method. From this analysis, reduction of energy barrier due to the interaction between dislocation and hydrogen atom is observed. Furthermore, stress field around a dislocation is investigated including the dislocation core structure based on atomic model.

ACKNOWLEDGEMENT

This research has been conducted as a part of "Fundamental Research Project on Advanced Hydrogen Science" funded by New Energy and Industrial Technology Development Organization (NEDO). And, this research was partially supported by the ENEOS Hydrogen Trust Fund, and the Ministry of Education, Science, Sports and Culture, Grant-in-Aid for Young Scientists (A), 2007

REFERENCES

[1] P. J. Ferreira, I. M. Robertson and H. K. Birnbaum, "Hydrogen effects on the character of dislocations in high-purity aluminum", Acta Mat., Vol. 47, 10, pp.2991-2998, (1999).

[2] H. K. Birnbaum, I. M. Robertson, P. Sofronis and D. Teter, "Mechanisms of hydrogen related fracture – a review", *Corrosion-deformation interactions*, T. Magnin, Inst. of Mat., pp.172-195, 1997.

[3] P. Sofronis and H. K. Birnbaum, "Mechanics of the hydrogen-dislocation-impurity", Mech. J. Phys. Solids, Vol. 43, 1, pp.49-90, (1995).

[4] S. Taketomi, R. Matsumoto and N. Miyazaki, "Atomistic simulation of the effects of hydrogen on the mobility of edge dislocation in alpha iron", J. Mat. Sci., accepted.