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

Atomistic Study of Interaction between Hydrogen Atoms and Dislocations around Mode I Crack Tip

***Ryosuke Matsumoto[1], Shinya Taketomi[2], Sohei Matsumoto[3], Yoshinori Inoue[4] and Noriyuki Miyazaki[5]**

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

[3] Graduate Student, Department of Mechanical Engineering and Science, Graduate School of Engineering, Kyoto University
Yoshida-Honmachi, Sakyo-ku, 606-8501 Kyoto, Japan
souhei@solid.me.kyoto-u.ac.jp
http://solid.me.kyoto-u.ac.jp

[4] Graduate Student, Department of Mechanical Engineering and Science, Graduate School of Engineering, Kyoto University
Yoshida-Honmachi, Sakyo-ku, 606-8501 Kyoto, Japan
inoue@solid.me.kyoto-u.ac.jp
http://solid.me.kyoto-u.ac.jp

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

Key Words: *Hydrogen Embrittlement, Molecular Dynamics, Crack Propagation, Brittle Fracture, Ductile Fracture, Dislocation, bcc-iron.*

ABSTRACT

There are great expectations to hydrogen as a next generation energy or a medium of energy. However, it is well known that hydrogen weakens the strengths of metals. For example, it decreases global elongation to failure and increases crack growth rate under cyclic loadings [1]. Despite the extensive investigations concerning hydrogen related fractures, the mechanisms have not been enough clarified yet. The difficulties to reveal the essential effects of hydrogen are mainly attributed to the characteristics of hydrogen such as ppm-order extremely low concentration, high diffusivity and high sensitivity to the defect-densities in metals. In this study, we performed molecular dynamics (MD) simulations of Mode I crack growth in bcc-Fe single crystals with and without hydrogen, and analyzed the hydrogen effects on the crack growth behavior from the atomistic viewpoints.

We used the quasi three dimensional models with a small thickness, and adopted the periodic boundary condition along the thickness direction. The models are composed of about 70,000 atoms whose interactions are described by the embedded atom method (EAM) potential developed by M. Wen et al.[2]. The multiple time step algorithm [3]

was also used as a time integration method. Recent detailed observations showed that hydrogen related fractures correlate closely with the dislocation motion. Consequently, the crack growth behaviors in two types of crystal orientation are analyzed. The first one has the crystal orientation in which dislocation emissions do not occur and the fracture type is brittle, and the other is directed to the crystal orientation in which dislocation emissions easily occur and the fracture type is ductile. In the case of the former crystal orientation, significant differences between models with and without hydrogen were not observed. However, in the latter case, it is revealed that simulation models with hydrogen are more likely to fracture along the slip planes than the models without hydrogen. We also show that the hydrogen atoms which are trapped by an edge-dislocation core distribute along the slip plane, and such a planar distribution of hydrogen leads to the slip plane fracture at the high dislocation density plane.

ACKNOWLEDGEMENTS

A part of this research is included in “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 Ministry of Education, Science, Sports and Culture, Grant-in-Aid for Young Scientists (A), 19686013, 2007.

REFERENCES

[1] Y. Murakami, “The effect of hydrogen on fatigue properties of metals used for fuel cell system”, *Int. J. of Fracture*, Vol. **138**, pp. 167-195, (2006).

[2] M.Wen, X.Xu, S.Fukuyama, K.Yokogawa, “Embedded-atom-method functions for the body-centered-cubic iron and hydrogen”, *J.Mater.Res.*, Vol. **16**, pp. 3496-3502, (2001).

[3] M.Tuckerman, B.J.Berne, G.J.Martyna, “Reversible multiple scale molecular dynamics”, *J.Chem.Phys.*, Vol. **97**, 1990-2001, (1992).