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

MOLECULAR DYNAMICS STUDY ON DISLOCATION ACTIVITIES IN IRON SPECIMENS INCLUDING HYDROGEN

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Key Words: *Molecular Dynamics, Hydrogen Embrittlement, Dislocation, Iron, Plastic Deformation.*

ABSTRACT

The influence of hydrogen atoms on dislocation activities near a crack tip in iron specimens has been examined using molecular dynamics (MD) simulations in order to establish the mechanism of hydrogen embrittlement. Our simulations revealed that the hydrogen atoms near the crack tip enhance dislocation emission from the crack tip due to the decrease of unstable stacking fault energy, as well as the hydrogen atoms in a slip plane decrease dislocation velocity, resulting in the slip plane decohesion.

Fuel cell system is a promissing technology as a clean enrgy for a next generation. To improve the reliability of the system, high-accuracy prediction of fracture under a hydrogen environment is needed. Despite a number of experimental studies [1, 2], the mechanisms of hydrogen embrittlement have not been clarified.

Cracked specimens used in this study consist of approximately 10000 iron atoms in a 90 Å x 90 Å x 14 $Å^3$ crystal in the *x*, *y* and *z* directions, corresponding to the $[11\bar{1}]$, $[1\bar{1}0]$ and [112] crystallographic directions, respectively. In the *y* direction, atoms in fixed boundary layers are deformed to apply shear stress to the specimens, whereas periodic boundary condition is imposed in the *z* direction. Temperature in the specimens keeps 300 K by means of velocity scaling method. The schematics of the simulated specimens including the hydrogen atoms are shown in Fig. 1.

Fig. 2 shows dislocation activities obtained from our MD simulations. Dislocation emission is accelerated by the hydrogen atoms around the stressed crack tip. The hydrogen atoms in the slip plane cause the reduction of dislocation velocity. In additon, it decreases with increasing hydrogen concentration.

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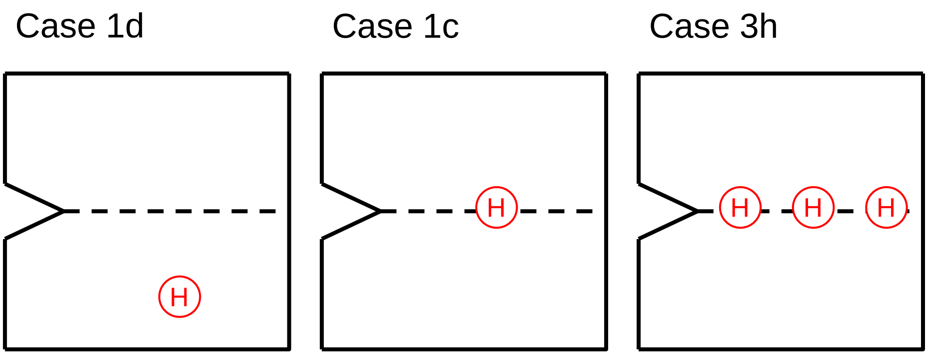

Fig. 1. The schematics of simulated specimens including hydrogen atoms subjected to shear stress are shown. Dotted lines indicate the slip plane of iron which corresponds to the (112) plane. For case 1d and case 1c, one hydrogen atom is placed down the slip plane and at the center of a specimen, respectively. For case 3h, three hydrogen atoms are placed in the slip plane horizontally.

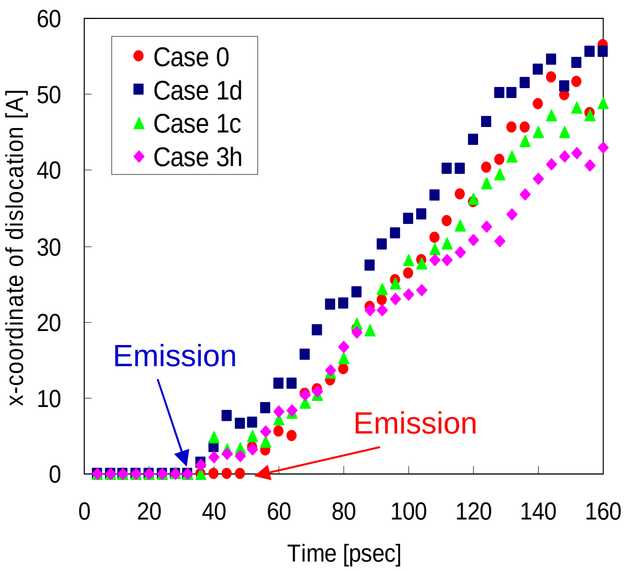

Fig. 2. The positions (x-coordinate) of a dislocation emitted from a stressed crack tip as a function of simulated time are shown. For case 0, a specimen does not include hydrogen atom. The dislocation velocity of case 0, case 1d, case 1c and case 3h estimated by the least-square method is 54.9, 53.1, 49.2 and 37.4 m/s, respectively. Dislocation emission in the specimens with hydrogen occurs earlier than the specimen without hydrogen. The hydrogen atoms in the slip plane obstruct dislocation motion.