11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

QM/MM ANALYSIS OF EFFECTS OF HYDROGEN AND HELIUM ON DISLOCATION MOTIONS IN BCC IRON

Ryo Kobayashi[1], Tomoyuki Tamura[2], and Shuji Ogata[3]

[1] Department of Scientific and Engineering Simulation, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan, kobayashi.ryo@nitech.ac.jp
[2] Center for Fostering Young and Innovative Researchers, Nagoya Institute of Technology
[3] Department of Scientific and Engineering Simulation, Nagoya Institute of Technology

Key words: *QM/MM simulation, Peierls barrier, bcc iron, nudged elastic band.*

Iron based materials are widely used in industrial field, such as frames of cars, ships, tankers, ships, pipelines in power plants, plasma facing walls of nuclear fusion reactors, etc. These materials are required to be hard, light, and tough. However it is known that hydrogen and helium often cause significant degradation of mechanical properties of these materials, for example, hydrogen embrittlement, hydrogen/helium induced voids, etc. It is important to understand the mechanism of these degradation phenomena for predicting material's lifetime and proposing new materials that have higher tolerance to hydrogen/helium emvironment. There have been a lot computational studies to investigate the effects of hydrogen and helium on iron-based materials using density functinoal theory (DFT) [1, 2] or classical molecular dynamics (MD) [2]. But, because large simulation cell and very accurate interatomic potential are required for the simulation of dislocation core structure, quantitative evaluation of migration barrier is difficult by either DFT or MD.

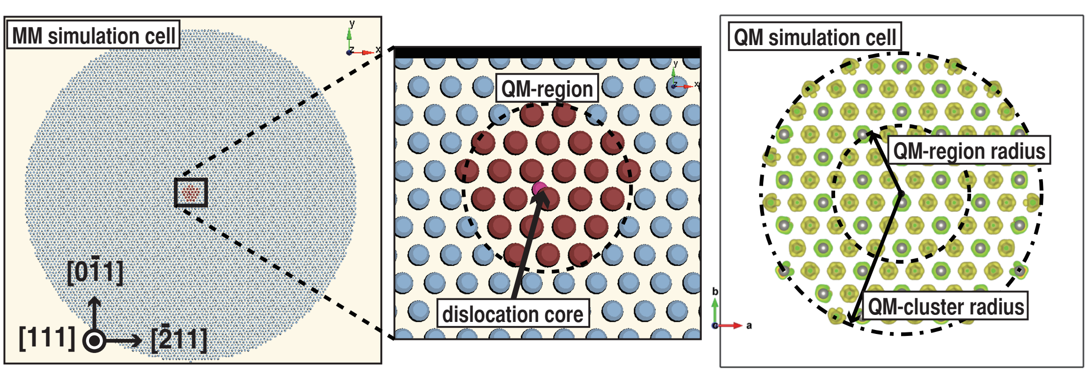

Figure 1: Schematic view of QM/MM model for screw dislocation in bcc iron. QM simulation cell includes buffer atoms and vacuum region.

In this paper, we have perform QM/MM simulation of migration of screw dislocation in bcc iron with or without hydrogen or helium. Using large simulation cell with periodic boundary condition along dislocation line and QM region only around the core (Fig. 1), we can calculate Peierls barrier of the screw dislocation with considering the elastic deformation field around the core by means of nudged elastic band method. We obtained the minimum energy path of dislocation migration with or without hydrogen or helium at hard-core or easy-core site (Fig. 2). Since helium atom has a large atomic radius and high dissolution energy, it is trapped at the dislocation core and the dislocation is also pinned vice versa. Hydrogen atom, on the other hand, works to both enhance and hinder depending on its position, hard-core or easy-core site. This is mostly because excluding volume effect of hydrogen and rooms at the dislocation core. Although the hard-core dislocation has higher energy than the easy-core dislocation because there are some short Fe-Fe bonds at the core, hydrogen at the hard-core site pushes those Fe atoms outward to have longer bond distances, resulting in the lower barrier of screw-dislocation migration. This variation of enhancement and hindrance by hydrogen depending on its position complicates the effects of hydrogen on dislocation motion. But, considering the binding energy of hydrogen and dislocation core, hydrogen tends to stay at the hard-core site next to the core and it works to enhance the dislocation motion.

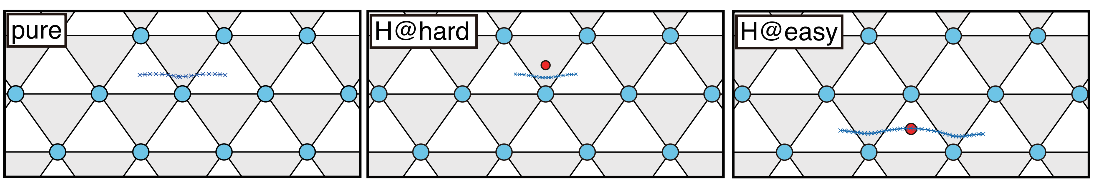

Figure 2: Migration paths with or without hydrogen at hard-core or easy-core on the paths.

REFERENCES

[1] M. Itakura, H. Kaburaki, and M. Yamaguchi, *First-principles study on the mobility of screw dislocations in bcc iron.* Acta Materialia, **60**, 3698—3710, (2012).

[2] L. Proville, L. Ventelon, D. Rodney, *Prediction of the kink-pair formation enthalpy on screw dislocations in α-iron by a line tension model parametrized on empirical potentials and first-principles calculations.* Physical Review B, **87**(14), 144106, (2013).