Monte Carlo simulations of Hydrogen trapping: adsorption/desorption kinetics

J. Sanchez*, A. Ridruejo† and J. Alonso†

* Instituto de Ciencias de la Construcción Eduardo Torroja (IETcc-CSIC)
Serrano Galvache 4, 28033, Madrid, Spain
e-mail: javier.sanchez@csic.es, web page: http://www.ietcc.csic.es

† Departamento de Ciencia de Materiales, Universidad Politécnica de Madrid, E.T.S.I. de Caminos, Canales y Puertos. Profesor Aranguren 3,28040, Madrid, Spain
Email: alvaro.ridruejo@upm.es - Web page: http://www.mater.upm.es

ABSTRACT

Hydrogen embrittlement is believed to be one of the main causes for cracking of steel structures under stress. Hydrogen absorbed in iron has been studied from different approaches, both from a theoretical and experimental point of view. Several mechanisms have been proposed to explain the behaviour and effect of hydrogen in the iron lattice, from hydrogen-enhanced localized plasticity to decohesion mechanisms. This behaviour is closely linked to hydrogen transport, which is modeled taking into account the effective diffusion coefficient, dependent on the trap density.

The present work studies the kinetics of hydrogen absorption with low energy traps. This kinds of traps represents a vacancy defect in the iron lattice. The methodology is based in Monte Carlo calculations. The results show the adsorption/desorption kinetics and establishes the equilibrium constant between the hydrogen in lattice and the hydrogen in traps. These parameters are also incorporated in a finite element model to simulate the effect of trap density in the crack propagation rate.

REFERENCES

[1] Sanchez, J., et al., Hydrogen in alpha-iron: Stress and diffusion. Physical Review B - Condensed Matter and Materials Physics, 2008. 78(1).
[2] Sanchez, J., et al., Ab initio molecular dynamics simulation of hydrogen diffusion in alpha-iron. Physical Review B - Condensed Matter and Materials Physics, 2010. 81(13).
[3] Castedo, A., et al., Ab initio study of the cubic-to-hexagonal phase transition promoted by interstitial hydrogen in iron. Physical Review B, 2011. 84(9): p. 094101.
[4] Sanchez, J., et al., Stress corrosion cracking mechanism of prestressing steels in bicarbonate solutions. Corrosion Science, 2007. 49(11): p. 4069-4080.
[5] Sanchez, J., et al., Measurement of hydrogen and embrittlement of high strength steels. Engineering Failure Analysis, 2016. 59: p. 467-477.
[6] Sanchez, J., J. Fullea, and C. Andrade, High Strength Steels Fracture Toughness Variation by the Media. Modelling of Corroding Concrete Structures, 2011. 5: p. 137-146.
[7] Elices, M., et al., Failure analysis of prestressed anchor bars. Engineering Failure Analysis, 2012. 24(0): p. 57-66.
[8] Serebrinsky, S., E.A. Carter, and M. Ortiz, A quantum-mechanically informed continuum model of hydrogen embrittlement. Journal of the Mechanics and Physics of Solids, 2004. 52(10): p. 2403-2430.
[9] Li, D.M., R.P. Gangloff, and J.R. Scully, Hydrogen trap states in ultrahigh-strength AERMET 100 steel. Metallurgical and Materials Transactions A-Physical Metallurgy and Materials Science, 2004. 35A(3): p. 849-864.
[10] Jiang, D.E. and E.A. Carter, Adsorption and diffusion energetics of hydrogen atoms on Fe(1 1 0) from first principles. Surface Science, 2003. 547(1-2): p. 85-98.
[11] Oriani, R.A., Mechanistic theory of hydrogen embrittlement of steels. Berichte Der Bunsen-Gesellschaft Fur Physikalische Chemie, 1972.