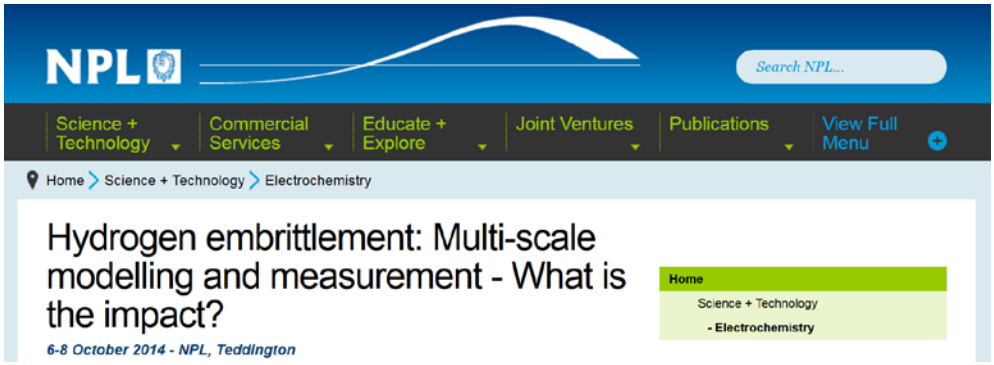

HYDROGEN EMBRITTLEMENT OF HIGH STRENTH STEELS: HYDROGEN INDUCED PHASE TRANSITION

J. Sanchez*, P. de Andres**, C. Andrade*, J. Fullea*

* *Instituto de Ciencias de la Construcción Eduardo Torroja (IETcc-CSIC). C/ Serrano Galvache, 4 - 28033 Madrid, Spain.*
** *Instituto de Ciencias de Materiales de Madrid (ICMM-CSIC). E-28049 Cantoblanco, Madrid, Spain.*

Hydrogen embrittlement is believed to be one of the main reasons for cracking of steel structures under stress and stress corrosion cracking process. To control and prevent the cracking of steel it is necessary to understand the chemical and physical properties of hydrogen inside iron.

Usually, pre-stressed steels are high strength steels that include a ferritic core made of α-iron (body-centered-cubic lattice, bcc). Previous works have focused on the effect of internal and external stresses/strains on the interstitial H and bcc-Fe interaction. Using ab-initio Molecular Dynamics and by taking statistical averages diffusion coefficients for hydrogen diffusion paths have been obtained. Depending on temperature, the diffusion path visits preferentially tetrahedral or octahedral sites. Simulations where a number of hydrogens occasionally meet in one unit cell have been performed to elucidate the effect of interactions between hydrogens, and diffusion coefficients have been calculated from Einstein´s equation. Under these conditions, the Fe-Fe interaction has been found to be weaker than in the absence of hydrogen. Debye temperature for Iron decreases monotonically with and increasing concentration of interstitial hydrogen, showing that iron-iron interatomic potential is weaker in the presence of a large number of diffusing hydrogen atoms.

In this work, we have focused on the structural consequences for the iron lattice upon absorption of interstitial H in octahedral sites. Using ab-initio Density Functional Theory we have computed the kinetic barriers for a phase transition bcc > fcc > hcp along a Bain's pathway. All the barriers are lowered by the presence of hydrogen; the initial part (bcc>fcc) being almost barrierless. This kind of phase transformation carries out atomic rearrangements and changes in the unit cell volume that should affect the mechanical properties of iron, as revealed by calculations for the elastic constants of the material.

REFERENCES

[1] A. Castedo, J. Sanchez, J. Fullea, M. C. Andrade, P. L. de Andres, Ab initio study of the cubic-to-hexagonal phase transition promoted by interstitial hydrogen in iron. Physical Review B 84, 094101 (2011).

[2] J. Sanchez, J. Fullea, M. C. Andrade, P. L. de Andres, Ab initio molecular dynamics simulation of hydrogen diffusion in alpha -iron. Physical Review B 81, 132102 (2010).

[3] J. Sanchez, J. Fullea, C. Andrade, P. de Andres, Hydrogen Embrittlement of High Strength Steels. Diffusion in Materials - Dimat2008 289-292, 203 (2009).

[4] J. Sanchez, J. Fullea, C. Andrade, P. L. d. Andres, Hydrogen in alpha-iron: Stress and diffusion. Physical Review B 78, 014113 (2008).