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

HYDROGEN EMBRITTLEMENT OF IRON BI-CRYSTALS

Nadia Salman[1], Malik A. Wagih[2], Tarek M. Hatem[3], Jaafar A. El-Awady[4]

[1] Department of Mechanical Engineering, British University in Egypt, Al-Shorouk, Cairo 11837 - P.O. Box 43, Egypt, nadia.salman@bue.edu.eg

[2] Department of Mechanical Engineering, British University in Egypt, Al-Shorouk, Cairo 11837 - P.O. Box 43, Egypt, malik.wagih@hotmail.com

[3] Department of Mechanical Engineering, British University in Egypt, Al-Shorouk, Cairo 11837 - P.O. Box 43, Egypt, tarek.hatem@bue.edu.eg

[4] Department of Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland 21218, USA, jelawady@jhu.edu

Keywords: *Martenstic Steel, Dislocation-Densities, Grain Boundary, Hydrogen Embrittlement*

One outstanding technological problem yet to be solved is the localization and failure of high-strength steel alloys due to hydrogen embrittlement. Hydrogen atoms affect the dislocation core causing the plastic deformation to localize and thus to decrease the material capacity for plastic deformation. Better understanding of the role of hydrogen will lead to reliable computational models that incorporate hydrogen effects and diffusion through dislocation-densities evolution laws.

Here we present large scale molecular dynamics simulations of the dislocation-density evolution and surface morphology in bi-crystal structure. The interrelated effects of size, GBs type and loading direction are investigated relative to the hydrogen concentration.