Atomistic simulation study on fatigue crack growth in Fe-Mn-C nanocrystals: Effect of deformation rate

Jaime A. Castañeda*, Manuel Camargo†

* Research Group on Fatigue and Surface (GIFS), Mechanical Engineering School
Universidad del Valle – Campus Meléndez
CALE 13 No 100-00, 760034 Cali, Colombia.

† Research on Energy and Materials (REM), Mechanical Engineering Faculty
Universidad Antonio Nariño (UAN), Campus Farallones
Km 18 vía Cali-Jamundí, 760030 Cali, Colombia
e-mail: jaime.castaneda@correounivalle.edu.co

e-mail: manuel.camarga@uan.edu.co

ABSTRACT

In the present work, molecular dynamic simulations were carried out to study the crack propagation in Fe-Mn-C nanocrystals, the damage behaviour in f.c.c. structure on the crack tip and the combinations of cleavage planes and dislocations slips systems. The effect of deformation rate and grain orientation on both the propagation mechanisms and glide planes is analyzed for different levels of stacking fault energy. Based on the MEAM potential, the interactions in Fe-Mn-C were fitting to reproduce the characteristics of crack propagation by comparing to experimental results from post mortem atomic force microscopy techniques. The system is modeled as a semi-infinite plate with either edge or center cracks subject to anisotropic displacements under failure mode I (K_I) for dynamic sinusoidal loads. The strength of the latter yields to stress intensity factors in the range (0.8 - 1.5) MPa*m^0.5. The proposed approach allows to determine the slow processes taking place in the crack tip, which can only be carried out at the nanoscale. It also predicts the mechanisms of micro-fracture for the Fe-Mn-C alloy, which open the panorama for future studies on complex alloys with applications in engineering complemented with continuous mechanics.

REFERENCES