Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1]Poster Session 1

Symposium E

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-27]Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient

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Delayed fracture in high-strength steel wires produced by drawing is an important issue. The major cause of the delayed fracture is supposed hydrogen embrittlement (HE), and some researches so far show that HE phenomena is very sensitive to the amount of plastic deformation in drawing process. The hydrogen(H)-atom diffusion is affected largely by ambient thermal and mechanical conditions, such as, stress, pressure and temperature. Besides, effect of stress gradient (SD) on atomic diffusion is supposed to be crucial, but is still unclear. Most of metallic materials which have been provided plastic deformation, like drawn pearlitic steel wires, have a enormous residual stresses particularly in surface and interface region, which shows strong SD. In this study, we investigate the behavior of H-atoms diffusing in pure iron (α-Fe) in the condition accompanied by SD. Since the behavior is observable just in atomic-scale, molecular dynamics (MD) simulation using EAM potentials for Fe and H atomic system is conducted. There are two types of SD condition: one is the gradient for overall specimen, which can be reproduced by bending deformation of specimen. Another is an atomic-scale gradient in the interface region, e.g. one provided by grain boundary (GB) structure. Thus, we build a bi-crystal model including GB structure, and it is applied bending deformation. For a moderate flexure, the bending stress distributes in a linear fashion along the lateral cross-section of the specimen. Diffusion coefficient of H-atoms in bulk region increases with increase of the SD value. Besides, it is clearly observed that the direction of diffusion depends on the distribution of SD. It is found that H-atom diffusion increases with the decrease of cohesive energy evaluated around the H-atom. From these MD results, we realize that the increase of H-atom diffusion shows exactly exponential relation to SD values. So, we can successfully obtain an expression between diffusion coefficient and SD value. We also understand that, by setting temperature effects aside, the increase of SD will lead to substantial change of entropy effect for diffusion.