Contribution ID: **452** Type: **Poster**

MOLECULAR DYNAMICS STUDY ON EFFECT OF GBS MISORITENTION ANGLE ON GBS HELIUM EMBRITTLEMENT IN BCC IRON

Wednesday 7 June 2017 13:40 (2 hours)

In fusion application, helium embrittlement is a key inducement to deteriorate mechanical performance of structural steels. To elucidate the mechanisms of helium induced embrittlement of grain boundaries (GBs), molecular dynamics (MD) was used to simulate GB tensile under the effect of helium bubbles in bcc iron at atomic level. Stress-strain curves and snapshots of configuration during tensile were extracted to analyze the mechanisms of GBs embrittlement. The GBs with <100> tilt axis and different misorientation angle which ranges from 5.5° to 84.5° were investigated under different helium concentration. Effect of misorientation angle on GB embrittlement was highlighted. The results indicate that the effect of helium bubbles on strength of GBs have significant dependency on misorientation angle of GBs. The study provides productive guidelines for the structural steels fabrication from the view of GB engineering.

Eligible for student paper award?

Yes

Author: SHI, Jingyi (University of science and technology of China)

Co-authors: PENG, Lei (University of Science and Technology of China); Dr GAO, Fei (University of Michigan); Prof. YE , Minyou (University of Science and Technology of China)

Presenter: SHI, Jingyi (University of science and technology of China)

Session Classification: W.POS: Poster Session W

Track Classification: Materials and fabrication