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Molecular Dynamics Study of Hydrogen Diffusion around a (112)[111] Edge Dislocation in Alpha Iron

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Summary

Despite the extensive investigations for over a century, the effects of hydrogen on material properties have not been clarified. The difficulties to reveal the essential effects of hydrogen are mainly attributed to the characteristics of hydrogen such as extremely low concentration and high diffusivity in metals. Therefore, the experimental estimation of the local hydrogen concentration around a dislocation, as well as the dislocation motion, is extremely difficult. Furthermore, it was experimentally and analytically confirmed that hydrogen enhances the dislocation mobility, and this mechanism is known Hydrogen Enhanced Localized Plasticity (HELP). However the local hydrogen distribution and the effects of the locally accumulated hydrogen have not been analyzed in spite of recent remarkable progresses in experimental equipments. In this study, we performed molecular statics (MS) simulations of hydrogen distribution around an (112)[111] edge dislocation in alpha iron single crystal. In this analysis, atomistic interactions are described by the embedded atom method (EAM) potential developed by M. Wen et. al. The results show that hydrogen concentrates to dislocation core and along the slip plane. Furthermore hydrogen trap energy shows asymmetrical distribution around the dislocation due to structural asymmetry of the (112)[111] edge dislocation in alpha iron. The stable hydrogen occupation region, where the hydrogen trap energy is strong, is not consistent with the result obtained by continuum theory of elasticity that hydrogen concentrate at the high hydrostatic stress region. According to the MS calculations, hydrogen trap energy changes under shear stress as well as hydrostatic stress. Moreover, hydrogen trap energy has different characteristics under shear stress even if a hydrogen atom exists at the same type of occupation site (Tetrahedral or Octahedral site). Thus, this results suggest that the hydrogen concentration on the slip plane around a (112)[111] dislocation, where the shear stress is high, can be extremely high.