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Molecular Dynamics Study of Hydrogen Effects on the Fracture Behavior of bcc-Fe Single Crystals

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Summary

It is well known that hydrogen weakens the strengths of metals, and this phenomenon is called "hydrogen embrittlement". Despite the extensive investigation concerning hydrogen-related fracture, the mechanism has not been enough clarified yet. The difficulties to reveal the essential effects of hydrogen are mainly attributed to the characteristics of hydrogen, namely, a ppm-order extremely low concentration, its high diffusivity and its high sensitivity to the defect-densities in metals. In this study, we applied molecular dynamics (MD) method to the mode I crack growth in the bcc-Fe single crystals with and without hydrogen, and clarified the hydrogen effects from the atomistic viewpoint. Recently detailed observations showed that hydrogen-related fractures correlate closely with the dislocation motion. Therefore, the crack growth behaviors are analyzed for two types of crystal orientations and compared with each other. The first one is directed to the crystal orientation, in which brittle fracture occurs without dislocation emission. The other is directed to the crystal orientation, in which ductile fracture occurs with dislocation emissions. In the case of the former crystal orientation, no significant difference is observed between the simulation models with and without hydrogen. On the other hand, it is revealed in the latter case that the simulation model with hydrogen is more likely to fracture along the slip planes than the model without hydrogen.