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Effect of irradiation and irradiation defects on the mobility of Σ5 symmetric tilt grain boundaries in iron: an atomistic study

X. Y. Wang[a], N. Gao[b], B. Xu[a,**], Y. N. Wang[a], G. G. Shu[c], C. L. Li[c], W. Liu[a,**]

[a]*School of Materials Science and Engineering, Tsinghua University, Beijing, 100084, PR China*
[b]*Laboratory of Advanced Nuclear Material, Institute of Modern Physics, 509 NanChang Rd. LanZhou 730000, PR China*
[c]*Sate Key laboratory of Nuclear power Safety Monitoring Technology and Equipment, China Nuclear Power Engineering Co., Ltd, Shenzhen 518172, China*

Abstract

Body center cubic iron materials are commonly used in nuclear power plants. In bcc-iron, symmetric tilt grain boundaries (STGBs), which are believed to play important roles on self-healing, are susceptible to configuration and structural change under irradiation. The effect of such changes on mechanical properties of such GBs is still unknown. In this work, using molecular dynamics simulations, we find that the critical shear stress τ_c required for Σ5 STGB migration is greatly reduced by either displacement cascade nearby or absorption of defect clusters. Moreover, we find that the trapping of radiation-induced interstitial-type dislocation loops could also decrease τ_c, indicating that displacement cascades could also exert a long-range effect on GBs due to the fast diffusion of interstitial clusters.

Keywords: Grain boundaries, Radiation Defects, Grain Growth, Stress and strain

*Corresponding author
**Corresponding author
Email addresses: xuben@mail.tsinghua.edu.cn, Tel:+8618611268045 (B. Xu), liuw@mail.tsinghua.edu.cn, Tel:+8601062772852 (W. Liu)