Atomistic interaction between grain boundaries and radiation-induced point defects in hcp titanium

Xiao Gao[a], Haixuan Xu[b], Simon R. Phillpot[c] and Man Yao[a,*]

[a] School of Materials Science and Engineering, Dalian University of Technology, Dalian, 116024,China

[b] Materials Science and Technology Division, Oak Ridge National Lab, Oak Ridge,TN,37831, USA

[c] Department of Materials Science and Engineering, University of Florida, Gainesville, FL 32611, USA

*Corresponding author: yaoman@dlut.edu.cn

TEL: +86-0411-84707347

FAX: +86-0411-8470928

Abstract:

The effect of grain boundaries (GBs) on radiation-induced point defects (vacancies and interstitials) were investigated in hcp titanium using molecular dynamics by creating the primary knock-on atom (PKA) at various distances from a GB. The average total number of point defects surviving in the grain region was compared with the results for single crystal. The results indicated that GBs act as sinks of radiation-induced point defects, with an efficiency depending on the degree of overlap between the GB and the cascade damage region. For a PKA of any given energy, there was an optimal distance from the GB, at which the number of residual radiation-induced point defects was minimized. For the low energies PKA explored here, this may result in a region of reduced concentration of defects near the GB.

Keywords：Radiation damage, Grain boundaries, point defects, Molecular dynamics, Ti