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

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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