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PROCEEDINGS

Molecular Dynamics Simulations of Displacement Cascade near Precipitate in Zirconium Alloys

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ABSTRACT

Precipitates play an important role in the evolution of irradiation-induced defects and mechanical property of irradiated metals. In this work, the effects of a Zr2Cu precipitate on the production and subsequent evolution of cascade-induced point defects (vacancies and interstitials) in ZrCu alloy were investigated by molecular dynamics simulations at room temperature. The simulation results show that the precipitate increases the number of residual point defects at the end of cascade. However, most of the residual defects reside in the precipitate and near precipitate boundary. In the matrix, more interstitials survive than vacancies. In addition, a defect-free region is seen in matrix and near precipitate boundary, indicating that the precipitate boundary traps vacancies/interstitials in matrix and retains them in the precipitate. To explain these observations, the formation energy and migration energy of point defects are calculated. The formation energies of both vacancy and interstitial decrease as they are moving to the precipitate boundary from matrix and precipitate, indicating that they can be absorbed by precipitate boundary and result in the defect-free region. However, the migration barrier of vacancy is lower than that of interstitial. Therefore, more vacancies in matrix are absorbed. The current work provides new insights into understanding the irradiation effects in zirconium alloys.

KEYWORDS

Zirconium alloy; precipitate; displacement cascade; point defect; molecular dynamics simulations

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