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Molecular dynamics simulations of high-energy displacement cascades in hcp-Zr

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Abstract

High-energy (up to 80 keV) displacement cascades in hcp-Zr are studied by classical Molecular Dynamics (MD) simulations. The statistics of defect production are reported and the formation of subcascades and defect clusters are analyzed. We find that the probability of subcascade formation increases along with the incident energy, and already reaches 100% at 80 keV. Our simulations also reveal that high-energy cascades could significantly promote the formation of defect clusters, sometimes even directly create experimental-scale (around 3 nm) vacancy clusters. Our research provides basic knowledge of high-energy displacement cascades in hcp-Zr, and offers a possible explanation for the low-dose irradiation experiments of Zr-based alloys.

Keywords: Molecular Dynamics, displacement cascades, high energy, Zr

1. Introduction

Zr-based alloys are widely-used structural materials in nuclear energy systems for their low neutron absorption, good mechanical strength, and adequate corrosion resistance[1]. However, it is well-known that neutron irradiation in nuclear reactors can induce heavy radiation damage in the alloys. In detail, the incident neutrons will introduce many energetic primary knock-on atoms (PKAs), which successively initiate atomic displacement cascades and produce numerous microscopic defects in the materials. On larger time scales, these retained defects will migrate, combine and evolve into complex defect clusters (such as voids, dislocation loops, etc), which finally lead to the degradation (swelling, hardening, embrittlement, etc) of the alloys' engineering properties. Although the whole damage process is a multiscale phenomenon (expanding from nm-ps to m-year)[2], most defects are produced by the PKAs, thus a comprehensive understanding of

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