

# 辐照诱导氢化钇损伤演化与变形行为

## 摘要

氢化钇是一种有望应用于先进微型反应堆的高温中子慢化剂，但其在亚化学计量氢含量条件下的辐照响应仍缺乏充分认识。本文采用透射电子显微镜 (TEM) 表征，并结合密度泛函理论 (DFT) 计算，系统研究了 YH<sub>1.58</sub> 在 2.5 MeV Fe<sup>2+</sup> 离子辐照条件下的微观结构演化行为，辐照温度范围为 50–465 °C，辐照剂量为 0.1 和 1.5 dpa。

在 0.1 dpa 条件下，辐照损伤主要表现为缺陷团簇，并呈现出明显的温度依赖性：随着辐照温度升高，缺陷团簇尺寸增大而密度降低；空洞仅在 465 °C 条件下可被观察到。在 1.5 dpa 条件下，损伤形貌发生显著变化，包括低温下微裂纹的形成以及较高温度下带状变形结构的出现。50 °C 条件下形成的开口微裂纹富集氧元素，这与氧化钇 (Y<sub>2</sub>O<sub>3</sub>) 的形成有关。DFT 计算表明，裂纹形成可产生由空位辅助的迁移通道，促进氢向裂纹表面迁移，从而推动氢脱附及后续氧元素掺入。

本研究揭示了温度、辐照剂量、变形行为与化学元素再分布在氢化钇辐照响应中的耦合作用，为理解氢化钇在先进核反应堆中的应用行为提供了新的认识。

## 关键词

氢化钇；离子辐照；微裂纹；微观结构演化

## Abstract

Yttrium hydride is a promising high-temperature neutron moderator for advanced microreactor applications, yet its irradiation response at substoichiometric hydrogen concentrations remains insufficiently understood. In this work, the microstructural evolution of YH<sub>1.58</sub> under 2.5 MeV Fe<sup>2+</sup> ion irradiation was systematically investigated over a wide range of temperatures (50–465 °C) and doses (0.1 and 1.5 dpa), using transmission electron microscopy (TEM), complemented by density functional theory (DFT) calculations. At 0.1 dpa, irradiation damage is dominated by defect clusters, with a clear temperature dependence: defect clusters increase in size and decrease in density as temperature rises, and cavities become observable only at 465 °C. At 1.5 dpa, pronounced changes in damage morphology are observed, including microcrack formation at low temperatures and band-shaped deformation structures at elevated temperatures. At 50 °C, open microcracks are oxygen-enriched due to the formation of yttrium oxide (Y<sub>2</sub>O<sub>3</sub>), with DFT calculations indicating that crack formation creates vacancy-assisted pathways that facilitate hydrogen migration towards crack surfaces, promoting hydrogen desorption and subsequent oxygen incorporation. These findings provide new insights into the coupled roles of temperature, irradiation dose, deformation, and chemical redistribution in the irradiation response of yttrium hydride, which is crucial for its application in advanced nuclear reactors.

## Keywords

Yttrium hydride; ion irradiation; microcracks; microstructural evolution

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