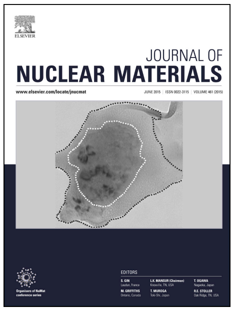

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# Quantifying the Stress State in the Vicinity of a $\delta$-Hydride in $\alpha$-Zirconium

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## Abstract

In zirconium alloys, precipitation of a hydride generally introduces internal stresses in the surrounding matrix. This study aims at understanding the role of internal stresses on the formation, growth and arrangement of $\delta$-hydrides in $\alpha$-zirconium. To this end, a Fast Fourier Transform based discrete dislocation dynamics technique is used to quantify both internal stresses induced during the formation of a hydride and the relief of the internal stresses by dislocation nucleation from the hydride-matrix interface. This work reveals that stress relaxation is localized in very small regions around the $\delta$-hydride ($\sim$ 300nm). Further, it is proposed that the dislocations nucleated from the hydride-matrix interface could act as loci for the nucleation of new hydrides, thereby rationalizing experimentally observed hydride stacks. Finally, quantifying the stress relaxation resulting from dislocation nucleation reveals that diagonal components of the internal stress inside the hydride remain very high, i.e., >3.0GPa. This suggests that additional dissipative processes, intrinsic to the hydride, are necessary to diminish the aforementioned internal stress.

*Keywords:* 3D discrete dislocation dynamics simulations, zirconium, hydride stacks, dislocation nucleation, internal stress fields

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## 1. Introduction

Zirconium (Zr) alloys are extensively used in the nuclear industry as clads for nuclear fuel in Light Water Reactors (LWR) as they show a good compromise of mechanical (e.g. high strength, ductility), chemical (e.g. excellent corrosion resistance) and nuclear (low absorption cross-section of thermal neutrons) properties [1]. One of the major drawbacks in the use of these alloys is the strong affinity of Zr for hydrogen. The water molecules surrounding the cladding reacts with the outer layer to form zirconium oxide and hydrogen (H) as by-product. As a consequence, H is absorbed into the Zr alloy cladding and forms zirconium hydride precipitates when the Terminal Solid Solubility (TSS) is surpassed [2, 3]. Although, the formation of hydrides in zirconium is a chemical process, it is essentially mechanically driven. In the absence of external stress, individual hydrides are reported to have size ranging from $10nm$ to $200nm$ (short radius of the hydrides)[4, 5]. Depending on the temperature and hydrogen content, hydrides are observed in one of four known hydride phases [4, 6]. The crystal structure and stoichiometric composition of each of these four phases are different [7]. The stable face-centered cubic (fcc) $\delta$-phase and the metastable face-centered tetragonal (fct) $\gamma$-hydride are the two commonly observed hydride phases in hexagonal close packed (hcp) zirconium. Due to the significant structural difference between the hydride phase and Zr matrix, elastic strain energy plays a dominant role in determining the hydride morphology [7]. Experimental observations revealed different morphologies for $\delta$-hydrides and $\gamma$-hydrides. $\delta$-hydrides were often observed to attain platelet-like morphology [8, 7, 5] and $\gamma$-hydrides resembled more like needles [9, 7]. Irrespective of the phase, these hydrides were mostly observed to align along the compact $\{11\bar{2}0\}$direction on the basal (0001) plane of the Zr matrix [10].

Precipitation of hydride induces a transformation strain. The internal stresses that are developed as a consequence are high enough to nucleate dislocations from the hydride-matrix interface into the

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