

Hydride Reorientation Under Normal Operating Conditions: Roles of Plastic Deformation and PCMI-Induced Hoop Stress

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1. Introduction

Hydride reorientation has traditionally been discussed mainly under dry storage conditions [1]. Since fission-gas release maintains a high rod internal pressure during the cooling process, tensile hoop stress can act on the cladding for an extended period. Recently, however, hydride reorientation has been reported in spent-fuel cladding [2]. As shown in Fig. 1, this observation suggests that reorientation may also occur under steady-state operating conditions.

This study proposes two factors that can trigger hydride reorientation under steady-state operating conditions. First, we focus on the role of accumulated plastic deformation in the cladding in reorientation behavior. As plastic deformation can accumulate beyond the elastic regime due to creep and pellet-cladding mechanical interaction (PCMI), this study aims to elucidate the mechanism by which plastic deformation promotes hydride reorientation. Second, we propose that hydride reorientation can be induced even under steady-state operation when tensile hoop stress is generated by PCMI, and we aim to validate this experimentally. Full-core fuel-performance calculations indicate that fuel rods with rod-average discharge burnup above ~50 MWd/kgU can experience local maximum tensile hoop stresses of ~100 MPa under steady-state PCMI, while the maximum cladding hydrogen concentration can exceed ~400 wppm [8]. These combined conditions—elevated tensile hoop loading and a substantial local hydrogen inventory—suggest that hydride reorientation may be possible even during normal operation. Through these efforts, this work aims to establish a basis for systematically assessing the potential for hydride reorientation during steady-state operation and to broaden the applicability of related cladding integrity evaluations.



Fig. 1. PIE-reported radial hydrides in spent-fuel cladding under normal operating conditions (adapted from [2], with permission).

2. Methods and Results

2.1 Sample preparation

Unirradiated, reactor-grade partially recrystallized annealed (PRXA) Zr-1.1Nb claddings with an outer diameter of 9.5 mm and thickness of 0.57 mm were used in these experiments. The chemical composition is summarized in Table 1.

Table 1: Chemical composition of the Zr-1.1Nb alloy

Elements	Zr	Nb	Cu
Wt%	Bal.	1.1%	0.05%

2.2 Experimental approach I : Hydride reorientation driven by plastic deformation

To minimize axial effects while introducing controlled and well-defined plastic deformation, ring specimens machined from a Zr-1.1Nb cladding tube were subjected to a ring compression test (RCT). Compression testing was conducted at room temperature using an Instron 8516 tensile-compression testing machine, and a total displacement of 4.4 mm was applied at a crosshead speed of 20 mm/min. After plastic deformation, the specimens were hydrogen charged at 400 °C, and the cooling rate was maintained at 0.5 °C/min during the subsequent cool-down process.

Following hydrogen charging, the specimens were mechanically polished for microstructural characterization. The polished specimens were etched in a mixed solution of water, nitric acid, and hydrofluoric acid in a 6:30:4 weight ratio, and then examined at 200× magnification using an optical microscope (OM; NIKON LV150N). Further microstructural and

crystallographic analyses were carried out using a field-emission scanning electron microscope (FE-SEM; MERLIN COMPACT) equipped with an EBSD system (Oxford Instruments Symmetry). For nanoscale examination of hydride morphology, site-specific lamellae were prepared by focused ion beam (FIB; FEI Helios 650) and analyzed by TEM (Thermo Fisher Scientific Themis Z).

2.3 Experimental approach II : Hydride reorientation under PCMI-induced tensile hoop stress

To identify hydride reorientation induced specifically by PCMI under steady-state operating conditions, it is necessary to prevent any additional reorientation from occurring during the cooling process. If reorientation also occurs during cool-down, it becomes impossible to distinguish whether the observed reorientation was formed during steady-state operation or newly induced during cooling. Therefore, to maintain a stress-free condition during the cooling interval, this study required an experimental setup that can maintain stress at high temperature and then remove it immediately at the onset of cooling. To implement this concept in a manner analogous to PCMI, a new mandrel apparatus was designed and fabricated.

The mandrel consists of three lower components and a triangular rod, as schematically illustrated in Fig. 2. A 1 cm-long Zr-1.1Nb cladding specimen was initially mounted in the loaded state shown in Fig. 2(a), with the triangular rod inserted to impose tensile hoop stress (PCMI analogue). The specimen was then heated to 400 °C, and hydrogen charging was performed for 24 hours while maintaining the applied stress at 400 °C. At the onset of cooling (cooling rate : 1°C/min), the chamber was shaken to release and remove the triangular rod, allowing the cladding to transition immediately to a stress-free condition, as shown in Fig. 2(b). The specimens were subsequently subjected to the mechanical polishing and etching procedures described in Section 2.2, followed by optical microscopy (OM) observation. The hydrogen concentration was measured using an ELTRA ONH-2000 analyzer. Finally, the radial hydride fraction (RHF) was quantified from the OM images using PROPHET.

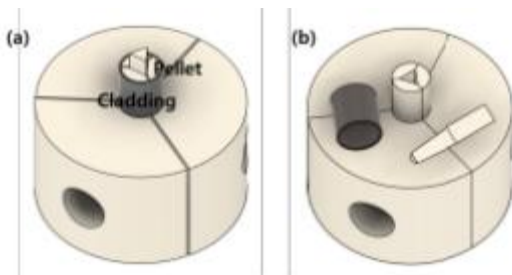


Fig. 2. Schematic of the custom mandrel apparatus for PCMI simulation: (a) stress-applied state prior to cooling and (b) stress-free state during cooling.

2.4 Result and interpretation I : Hydride reorientation driven by plastic deformation

OM images of the specimens following RCT and hydrogen charging are shown in Fig. 3. Hydride reorientation occurs in the compressed specimens at the 12 and 6 o'clock positions on the outer surface and at the 3 and 9 o'clock positions on the inner surface.

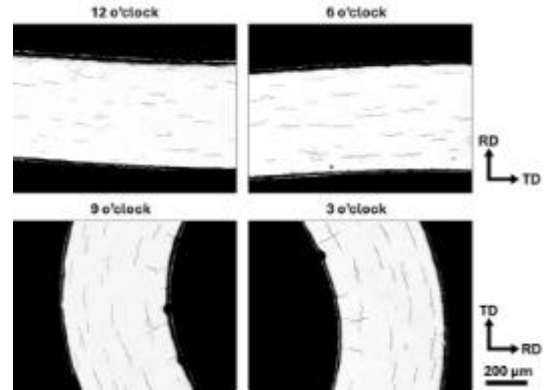


Fig. 3. Optical micrographs of the cladding after ring compression testing (RCT) and hydrogen charging, taken at the 12, 3, 6, and 9 o'clock positions.

Subsequently, the hoop stress distribution during the RCT was evaluated using ANSYS software. As shown in Fig. 4(a), all locations where hydride reorientation was observed shared the common feature that they were subjected to compressive hoop stress. To examine the microstructural influence of compressive hoop stress, EBSD analyses were conducted on the inner and outer surfaces at the 12 o'clock and 3 o'clock positions. The results indicate that the regions under compressive hoop stress—namely, the outer surface at 12 o'clock and the inner surface at 3 o'clock—exhibited a more pronounced tilting of the (0001) basal plane toward the RD direction, as shown in Fig. 4(b). This behavior is interpreted as a consequence of plastic deformation-induced lattice rotation during the RCT process.

Shi et al. (2024) reported that multiple slip systems can be activated even at room temperature in polycrystalline zirconium, indicating possible contributions not only from prismatic $\langle a \rangle$ slip but also from basal $\langle a \rangle$ slip and pyramidal $\langle a \rangle$ slip [3]. In addition, simulations of texture evolution by Chapuis and Liu (2015) showed that basal $\langle a \rangle$ slip and pyramidal $\langle a \rangle$ slip tend to rotate the c-axis toward the compression direction [4]. Therefore, the RD-directed tilting of the basal pole observed in this study is considered to be consistent with lattice rotation under compressive hoop stress.

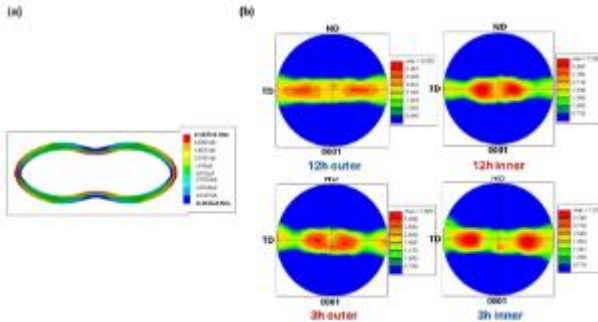


Fig. 4. (a) ANSYS-simulated hoop-stress distribution of the cladding during RCT at a compression displacement of 4.4 mm. and (b) (0001) basal pole figures measured by EBSD at the 12 and 3 o'clock positions.

Considering that hydride reorientation was observed only in regions where the basal plane is tilted toward the RD direction, the basal-plane orientation is suggested to play an important role in hydride precipitation and reorientation behavior. To examine this possibility, EBSD analyses were conducted on radial and circumferential hydrides located at the 3 o'clock inner-wall position.

Figure 5(a) presents an IPF map of the α -Zr matrix, in which the δ -hydride phase is overlaid in yellow. The red lines correspond to interface traces determined from the commonly reported α -Zr/ δ -hydride OR, $(0001)_\alpha // \{111\}_\delta$. Quantitative assessment confirmed that 68.2% of the observed interfaces are consistent with this OR. Figure 5(b) presents the (0001) pole figure constructed from all α -Zr grains within the region shown in Fig. 5(a), whereas Fig. 5(c) shows the (0001) pole figure for only those α -Zr grains that directly contact the δ -hydrides and form the interfaces in Fig. 5(a). The 3 o'clock inner-wall region exhibited pronounced basal-pole tilting across the overall α -Zr grain population, likely due to plastic deformation introduced during the RCT process. The α -Zr grains adjacent to radial hydrides were also predominantly composed of grains exhibiting similarly strong basal-pole tilting.

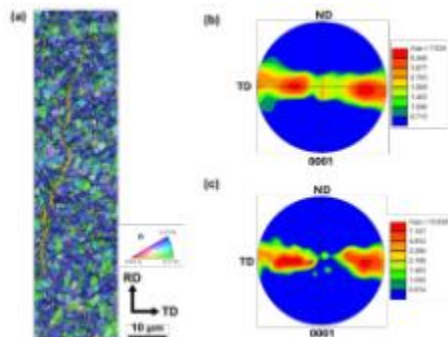


Fig. 5. EBSD analysis of radial hydrides at the 3 o'clock inner-wall region. (a) IPF map with δ -hydrides (yellow), (b) (0001) pole figure of all α -Zr grains in (a), (c) (0001) pole figure of hydride-adjacent α -Zr grains in (a).

Next, EBSD analyses were performed on the circumferential hydrides present at the 3 o'clock inner-wall position. Figure 6(a) presents an IPF map of the α -Zr matrix, in which the δ -hydride phase is overlaid in yellow. The red lines correspond to interface traces determined based on the commonly reported orientation relationship (OR) at the α -Zr/ δ -hydride interface, $(0001)_\alpha // \{111\}_\delta$. Quantitative assessment confirmed that 69.2% of the observed interfaces are consistent with this OR. Figure 6(b) shows the (0001) pole figure constructed from all α -Zr grains within the region shown in Fig. 6(a), whereas Fig. 6(c) shows the (0001) pole figure constructed using only the α -Zr grains that directly contact the δ -hydrides and form the interfaces in Fig. 6(a).

As the circumferential hydrides are located farther from the inner surface than the radial hydrides, the α -Zr grains in this region exhibit a smaller overall degree of basal-pole tilting. While the $\{0001\}$ poles of the overall α -Zr grain population in Fig. 6(b) are broadly distributed, those of the hydride-adjacent α -Zr grains are markedly concentrated toward TD (Fig. 6(c)). In other words, despite the diverse orientation distribution of the overall grain population, circumferential hydrides form selectively in grains whose basal planes are oriented close to TD. Furthermore, when considered together with the observation that plastic-deformation-induced hydride reorientation occurs in regions where the basal plane is tilted toward the RD direction, these results strongly support that the basal-plane orientation is a key governing factor for both hydride precipitation.

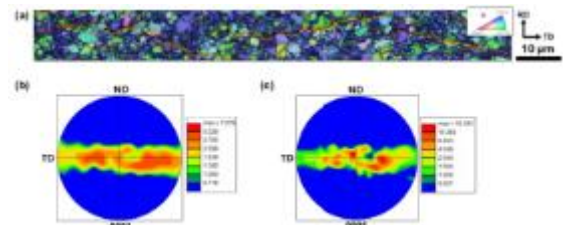


Fig. 6. EBSD analysis of circumferential hydrides at the 3 o'clock inner-wall region. (a) IPF map with δ -hydrides (yellow), (b) (0001) pole figure of all α -Zr grains in (a), (c) (0001) pole figure of hydride-adjacent α -Zr grains in (a).

The basal plane plays an important role in hydride precipitation primarily because the hydride/matrix interface is crystallographically constrained by the α -Zr/ δ -hydride orientation relationship (OR). In the α -Zr/ δ -hydride system, the dominant OR is most frequently reported as $(0001)_\alpha // \{111\}_\delta$ together with $\langle 11\bar{2}0 \rangle_\alpha // \langle 110 \rangle_\delta$. Under this OR, δ hydrides precipitate as platelets whose broad-face habit plane aligns close to $(0001)_\alpha$, such that the matrix basal texture effectively guides hydride alignment [5]. With mesoscale growth, the transformation misfit is accommodated by misfit dislocations and dislocation emission, leading to coherency loss and the development of an incoherent interface [6].

Nevertheless, even after coherency is lost, the interface remains crystallographically anchored by the OR and therefore tends to form close to the basal plane.

TEM was employed to examine the radial hydride located at the inner surface in the 3 o'clock direction. Figure 7(a) shows a BF image of the radial hydride, where the white line indicates the interface between the hydride and the parent α -Zr matrix. In this viewing orientation, the $[110]$ zone axis of the hydride is aligned with the $[11\bar{2}0]$ zone axis of the α -Zr matrix. The corresponding SAED patterns (Fig. 7(b) and (c)) include diffraction reflections from both the Zr matrix and the hydride phase, confirming the OR of $[11\bar{2}0]_{\alpha} // [110]_{\delta}$ and $(0001)_{\alpha} // \{111\}_{\delta}$. In addition, the observed interface is aligned with $\{10\bar{1}3\}_{\alpha} // \{110\}_{\delta}$. These results suggest that the radial hydride follows the dominant OR during precipitation and growth and subsequently develops an incoherent interface.

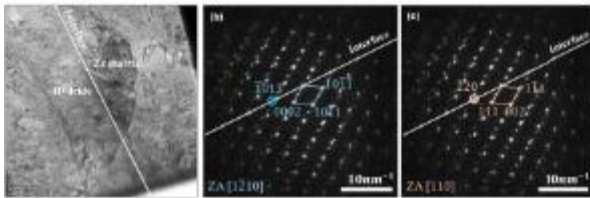


Fig. 7. (a) Bright-field (BF) TEM image of a radial hydride at the inner surface (b,c) Corresponding composite SAED patterns acquired across the interface, showing zone axes of (b) α -Zr $[11\bar{2}0]$ and (c) hydride $[110]$

These results show that plastic deformation can tilt the α -Zr basal plane and thereby promote hydride reorientation. This suggests that basal-plane tilting caused by in-reactor deformation, such as creep or PCMI-driven local plasticity, could also lead to reorientation during normal operation and therefore warrants systematic assessment.

2.4 Result and interpretation II : Hydride reorientation under PCMI-induced tensile hoop stress

Mandrel testing was conducted to apply a hoop stress exceeding the critical threshold (more than 200 MPa based on ANSYS estimations), and the specimens were hydrogen-charged to a total concentration of 479 ppm at 400 °C for 24 h. At the onset of cooling, the triangular loading rod was removed to immediately release the applied stress. The OM observation results are presented in Fig. 8(a). The radial hydride fraction (RHF) was quantified from the OM images using PROPHET, and the result is shown in Fig. 8(b). The measured RHF was 15.01%, indicating the formation of a substantial amount of radial hydrides. By applying the RHF to the total hydrogen concentration, the corresponding hydrogen amount for radial hydrides is estimated to be 71.85 ppm.

Based on the terminal solid solubility for precipitation (TSSP) of Zr-1.1Nb reported by Kim et al.

[7], the TSSP at 400 °C is approximately 390 ppm. As the total hydrogen concentration in this study (479 ppm) exceeds this value, hydride nucleation is considered to have initiated during the 400 °C holding period. Notably, the observation of radial hydrides in this experiment suggests that hydride reorientation can occur under normal operating conditions when the cladding experiences hoop stress above a critical level due to PCMI. However, because the specimens were transitioned to a stress-free condition during cooling, circumferential hydride formation is expected to have been relatively favored during cooling, which may explain the relatively low final RHF.

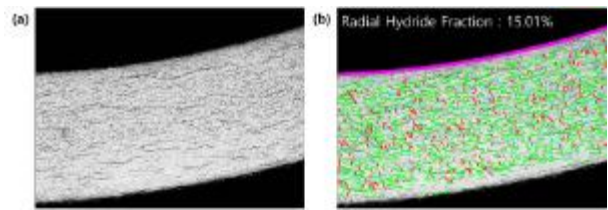


Fig. 8. (a) OM image of the cladding after hydrogen charging at 400 °C under mandrel-imposed hoop stress, (b) PROPHET-based RHF analysis result from the OM image

This study shows that hydride reorientation can occur under normal operating conditions when PCMI imposes a hoop stress exceeding a critical level. According to Lee et al., the local maximum hoop stress can exceed 100 MPa in most PWRs, and soluble boron-free (SBF) SMRs may experience locally intensified PCI due to reactivity control by control rods [8]. Therefore, PCMI-induced hydride reorientation under normal operating conditions may occur in many PWRs, and it should be considered with particular emphasis for SBF SMRs.

3. Conclusions

This study shows that hydride reorientation can occur even under steady-state operating conditions and experimentally validates two contributing factors. First, accumulated plastic deformation in the cladding (e.g., due to creep and PCMI) induces lattice rotation that tilts the α -Zr (0001) basal plane, and such basal-plane tilting can promote reorientation. Second, when PCMI generates a tensile hoop stress exceeding a critical level, reorientation can be induced, as verified using a mandrel-based experiment.

In the plastic-deformation-based approach (I), Zr-1.1Nb ring specimens were subjected to ring compression testing (RCT) to introduce controlled plastic deformation while minimizing axial effects, followed by hydrogen charging at 400 °C. OM observations revealed hydride reorientation at specific clock positions, and ANSYS analysis confirmed that these locations were commonly subjected to compressive hoop stress. EBSD results showed that the reoriented regions exhibited a stronger RD-directed tilting of the α -Zr (0001) basal pole, consistent with lattice rotation associated with activation of multiple

slip systems during plastic deformation. EBSD comparisons of radial and circumferential hydrides further confirmed that basal-plane orientation is a key factor governing hydride precipitation. This originates from the dominant α -Zr/ δ -hydride orientation relationship, $(0001)_\alpha // \{111\}_\delta$ and $\langle 11\bar{2}0 \rangle_\alpha // \langle 110 \rangle_\delta$, which crystallographically constrains the interface to form close to the basal plane. TEM/SAED also confirmed the same OR, supporting the interpretation that the observed hydrides grow while maintaining the dominant OR and subsequently develop an incoherent interface. Accordingly, it should be examined whether in-reactor deformation, such as creep and PCMI, induces basal-plane tilting that could drive hydride reorientation.

In the PCMI-based approach (II), a custom mandrel apparatus was designed and fabricated to eliminate additional reorientation during cooling by maintaining the applied stress up to 400 °C and then removing it immediately at the onset of cooling. Under a hoop stress condition estimated by ANSYS to exceed 200 MPa, specimens were hydrogen-charged to a total concentration of 479 ppm at 400 °C for 24 h. Radial hydrides were observed by OM, and PROPHET-based analysis quantified an RHF of 15.01%. As the total hydrogen concentration in this study (479 ppm) exceeds the reported TSSP of Zr-1.1Nb at 400 °C (~390 ppm), hydride nucleation had already initiated during the 400 °C holding period. The observation of radial hydrides under these conditions suggests that reorientation can be induced under normal operating conditions when PCMI generates a tensile hoop stress above a critical level.

Furthermore, considering reports that the local maximum hoop stress can exceed 100 MPa in most PWRs, PCMI-induced hydride reorientation during normal operation may occur in many PWRs. In particular, soluble boron-free (SBF) SMRs may experience locally intensified PCI due to control-rod-driven reactivity control. Therefore, the potential for reorientation during normal operation and its implications for cladding integrity should be considered with particular emphasis for SBF SMRs.

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