Oral presentation | V. Nuclear Fuel Cycle and Nuclear Materials：502-1 Nuclear Materials, Degradation, Radiation Effects, and Related Technology

Fri. Sep 13, 2024 10:15 AM - 11:55 AM JST | Fri. Sep 13, 2024 1:15 AM - 2:55 AM UTC Room O(Recture RoomsB 2F B204)

[3O01-06] Cladding Materials 1

Chair:Shinichiro Yamashita(JAEA)

10:15 AM - 10:30 AM JST | 1:15 AM - 1:30 AM UTC

[3O01]

Irradiation behavior of alumina scales formed on FeCrAl ODS alloys and the effect of pre-oxidation temperatures

*Hao Yu[1], Sosuke Kondo[1], Yasuyuki Ogino[1], Minha Park[1], Ryuta Kasada[1] (1. Tohoku Univ.)

10:30 AM - 10:45 AM JST | 1:30 AM - 1:45 AM UTC

[3O02]

Suppression of irradiation hardening in W-coated F82H produced by underwater explosive-welding

*Kotaro Seki[1], Kazuyuki Hokamoto[2], Shigeru Tanaka[2], Takaaki Koyanagi[3], Kenta Yoshida[1], Akira Hasegawa[1], Sosuke Kondo[1], Hao Yu[1], Yasuyuki Ogino[1], Ryuta Kasada[1,4] (1. Tohoku Univ., 2. Kumamoto Univ., 3. Oak Ridge National Laboratory, 4. National Institute for Fusion Science)

10:45 AM - 11:00 AM JST | 1:45 AM - 2:00 AM UTC

[3O03]

Microstructural Evolution and Interface Stability of Cr/Mo-Coated Zirconium Alloys Near the Mo-Zr Eutectoid Temperature

*BO LI[1], Jingjie Shen[3], Zongda Yang[1], Kano Sho[2], Hiroaki Abe[1] (1. UTokyo, 2. QST, 3. NIFS)

11:00 AM - 11:15 AM JST | 2:00 AM - 2:15 AM UTC

[3O04]

High-Temperature Air Oxidation Behavior of Cr-based Binary Alloys

*John Andrew Kane Jovellana[1], Hiroaki Abe[1] (1. UTokyo)

11:15 AM - 11:30 AM JST | 2:15 AM - 2:30 AM UTC

[3O05]

Evaluation of the Hoop Tensile Behavior of Cr-coated Zircaloy-4 Fuel Cladding by Advanced Expansion Due to Compression (A-EDC) Test

*Ziqi Wei[1], Bo Li[1], Lijuan Cui[3], Zongda Yang[1], Risheng Qiu[1,4], Sho Kano[2], Hiroaki Abe[1] (1. The University of Tokyo, 2. QST, 3. Sichuan Univ., 4. Chongqing Univ.)

11:30 AM - 11:45 AM JST | 2:30 AM - 2:45 AM UTC

[3O06]

Development of potential function for SiC materials used in nuclear applications based on machine learning

*Baopu WANG[1], Liangfan Zhu[1], Yuting Chen[1], Hirotomo Iwakiri[2], Kazunori Morishita[1] (1. Kyoto Univ., 2. Ryukyus Univ.)

11:45 AM - 11:55 AM JST | 2:45 AM - 2:55 AM UTC

Time reserved for Chair

Irradiation behavior of alumina scales formed on FeCrAl ODS alloys and the effect of pre-oxidation temperatures

*Hao Yu[1], Sosuke Kondo[1], Yasuyuki Ogino[1], Minha Park[1] and Ryuta Kasada[1]
[1]Tohoku Univ.

Abstract

Alumina-forming FeCrAl ferritic oxide dispersion strengthened (ODS) alloys are considered to be promising materials for nuclear systems. Present work aims to investigate the irradiation behavior of the alumina scales formed on FeCrAl ODS alloys at various pre-oxidation temperatures. Influence of microstructure control through adjusting the pre-oxidation temperatures on the irradiation resistance will be discussed.

Keywords: FeCrAl ODS, Alumina, Irradiation, Pre-oxidation

1. Introduction

The most appealing aspect of the FeCrAl ODS alloys is the ability to spontaneously form a dense α-alumina scale upon exposure to high temperatures, which can protect the alloys from extremely high temperature steam in accidental nuclear environments. Improving the radiation resistance of the alumina scale is essential for nuclear applications. Since the microstructure of the alumina scales is closely related to the temperature [1], in order to understand the role of microstructural control on the improvement of the irradiation resistance of the alumina scales, the irradiation behavior of alumina scales formed at different temperatures has been investigated.

2. Experimental

The alumina scales formed on different pre-oxidation temperatures were characterized by SEM, EPMA and XRD. The pre-oxidized FeCrAl ferritic ODS alloys were irradiated using a 6.4 MeV Fe^{3+} ion beam to 2 dpa at 500 °C in DuET, Kyoto University. Effect of the irradiation on the microstructure of the alumina scales was elucidated with the aid of STEM and 3D-AP characterization techniques. Evolution of the mechanical performance of the alumina scales before and after the irradiation was investigated by means of ultra-small testing technologies (USTT).

3. Result

Fine Y-Zr oxide particles were found in the formed alumina scale, which were originally existed in the alloy substrate and subsequently incorporated into the alumina layer with the inward growth of the alumina. As the pre-oxidation temperature increases, the Y-Zr oxide particles within the alumina layer show a tendency to diffuse from the metal substrate to the gas interface of the scale. The irradiation-induced segregation of Y/Zr along the alumina grain boundaries (G.B.) was confirmed, resulting in a reduction of alumina grain boundary cohesion.

4. Conclusion

Microstructural control by adjusting the pre-oxidation temperature contributes to the microstructural stability of alumina scales during irradiation, especially the distribution of the Y-Zr oxide particles, which provides the possibility to improve the irradiation resistance of the alumina scales.

References

[1] H. Yu, S. Kondo, R. Kasada, N. Oono, S. Hayashi, S. Ukai, Nucl. Mater. Energy 25 (2020) 100798

水中爆接法で作製した W/F82H 被覆材における照射硬化の抑制現象

Suppression of irradiation hardening in W-coated F82H produced by underwater explosive-welding

*関 航太朗[1], 外本 和幸[2], 田中 茂[2], 小柳 孝彰[3], 吉田 健太[1], 長谷川 晃[1], 近藤 創介[1], 余 浩[1], 荻野 靖之[1], 笠田 竜太[1,4]

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本研究は、水中爆接法によって作製した W/F82H 被覆材の機械特性に及ぼす中性子照射の影響を明らかにすることを目的する。W/H82H 被覆材の界面近傍における中性子照射前後でのビッカース硬さ変化を評価した結果、照射硬化の抑制が確認され、爆接時に導入された歪みの緩和が原因であると示唆された。

キーワード： 水中爆接，タングステン被覆，中性子照射，照射硬化，ビッカース硬さ試験

1. 背景・目的

核融合炉ブランケットの第一壁材料として、基材となる低放射化フェライト鋼にタングステン材料を被覆した W/F82H 被覆材が開発され、熱伝導特性や機械特性について研究されている。しかし、中性子照射後の W/F82H の機械特性に関する知見は多くない。本研究では、水中爆接材における中性子硬化を調べ、W/F82H 及びそれらの界面の照射硬化感受性に及ぼす接合の影響を明らかにすることを目的とした。

2. 実験方法

水中爆接法で作製した 3×3×3mm の W/F82H に対して中性子照射を実施した。硬さ試験はビッカース試験及びナノインデンテーションを行った。ビッカース硬さ試験は、荷重 980mN、保持時間 15 秒とした。ナノインデンテーションは、荷重 30mN、ステップサイズ 7μm とした。微細組織観察・解析は電子線後方散乱回折(EBSD)法、電子プローブマイクロアナライザー(EPMA)及び WB-STEM を用いた。中性子照射は BR2 及び HFIR を用いた。BR2 では、照射温度 100～150 及び 290℃とし、最大照射量を 1.27×10^{24}[/m^2]とした。HFIR では、照射温度 600℃とし、最大照射量を 21.5×10^{24}[/m^2]とした。

3. 結果・考察

未照射材に対するビッカース硬さ及びナノインデンテーション結果より、W/F82H はタングステン領域、界面領域、F82H 領域に加えて、F82H 硬化領域(Under-Clad Hardened : UCH 領域)の 4 種類の領域に分けられることが確認された。EMPA 解析結果より UCH 領域は F82H 領域と顕著な差は見られなかったが、EBSD 結果より UCH 領域は F82H 領域より測定不能領域が多く、高い歪みを有することが示唆された。また、硬さ試験後の W/F82H 界面領域には亀裂が確認されなかったが、タングステン領域の結晶粒界には亀裂が生じる傾向にあり、界面強度はタングステンの粒界強度よりも高い傾向にあることが示された。

中性子照射前後の硬さと比較すると、全ての領域で照射による硬化が抑制されていた。一方で、WB-STEM よりタングステン領域及び界面領域には照射欠陥が導入されていることが確認されたため、照射による硬化と同時に軟化が起こっていることが示唆された。照射による軟化の原因は、水中爆接によって導入された加工硬化あるいは弾性歪みが照射によって緩和したことであると示唆された[1]。

参考文献 [1]Fujii K, et al. *J Inst og Nucl Saf Syst.* 2011;18:198-210.

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*Kotaro Seki[1], Kazuyuki Hokamoto[2], Shigeru Tanaka[2], Takaaki Koyanagi[3], Kenta Yoshida[1], Akira Hasegawa[1], Sosuke Kondo[1]. Hao Yu[1], Yasuyuki Ogino[1], Ryuta Kasada[1,4]

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Microstructural Evolution and Interface Stability of Cr/Mo-Coated Zirconium Alloys Near the Mo-Zr Eutectoid Temperature

*Bo Li[1], Jingjie Shen[2], Zongda Yang[1] Sho Kano[3] and Hiroaki Abe[1]

[1] UTokyo, [2] NIFS, [3] QST

Abstract

This study is concerned with the interfacial evolutionary behavior of the Cr/Mo-coated Zr alloy, an accident-tolerant fuel cladding tube. The interfacial microstructure of Cr/Mo-coated Zr alloy and the mechanism of its formation were investigated at three temperatures: 700, 750, and 800 °C.

Keywords: ATF, Interface, Microstructure

1. Introduction

Zirconium (Zr)-based alloys have been employed as nuclear fuel cladding materials due to their low thermal neutron capture cross-section and oxidation resistance. The 2011 Fukushima Daiichi accident exposed the rapid oxidation and failure of Zr alloys at high temperatures, leading to hydrogen explosions. To enhance the accident tolerance of cladding tubes, particularly under LOCA conditions, Cr coatings on Zr cladding have emerged as a promising solution due to their robust corrosion resistance. However, the Cr/Zr interface's stability is challenged by interdiffusion, forming brittle ZrCr2 compounds and potential Cr-Zr eutectic reactions above 1330°C. Various barrier layers, including Molybdenum (Mo), have been explored to mitigate these issues. Mo is particularly promising due to its thermal properties and higher eutectic temperature with Zr. Prior studies have focused on high-temperature performance, but the behavior around the Mo-Zr eutectoid temperature (~750°C) remains less understood. This study investigates the microstructural evolution of Cr/Mo-coated Zr alloys in the 700-800°C range, focusing on the interface before and after the eutectoid reaction, aiming to enhance the safety margin of these cladding tubes.

2. Experimental process and results

Cr/Mo-coated Zr alloys were fabricated using pulsed laser deposition (PLD). The samples were annealed at three different temperatures: 700 °C, 750 °C, and 800 °C, each for 4 hours in a high vacuum environment. After annealing, the samples were cooled to room temperature within the furnace. Subsequently, specimens subjected to different heat treatments were prepared using a focused ion beam (FIB) and examined with a transmission electron microscope (TEM) equipped with an energy-dispersive spectrometer (EDS). This allowed us to analyze the microstructure and compositional distribution at the Cr/Mo-coated Zr alloy interfaces under various heat treatment conditions.

The results indicate that Mo serves as an effective diffusion barrier below 750 °C, preventing the formation of intermetallic compounds in the interfacial region. However, once the temperature reaches 750 °C, which is above the Mo-Zr eutectoid reaction temperature, significant reactions between Mo and Zr occur. This leads to the formation of four distinct phases in the interfacial region, including a large intermetallic compound, $Zr(Mo, Cr, Fe)_2$.

3. Conclusion

This study examined the microstructural evolution and composition distribution at Cr/Mo-coated Zr alloy interfaces near the Mo-Zr eutectoid temperature (700-800 °C). 730 °C, Mo effectively acts as a diffusion barrier, preventing intermetallic compound formation. However, above this temperature, Mo loses its barrier function, leading to the development of four distinct interfacial zones: β-Zr, large $Zr(Mo,Cr,Fe)_2$ intermetallic compounds, α-Zr, and the original Mo layer with fine $Zr(Mo,Cr,Fe)_2$, severely impacting interface performance.

High-Temperature Air Oxidation Behavior of Cr-based Binary Alloys

*John Andrew Kane Jovellana[1] and Hiroaki Abe[1]

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ATF research currently focus on Cr-based coatings to protect Zr alloys. However, it is necessary to improve Cr properties via alloying. In this study, Cr alloys with Fe and Al are prepared by arc melting. Weight gains after furnace oxidation are compared, and morphology and oxides composition after air oxidation were analyzed. The oxidation resistance of the Cr-Fe and Cr-Al alloys are considered to be satisfactory.

Keywords: ATF, chromium, oxidation

1. Introduction

As a severe consequence of Fukushima Daiichi nuclear accident, the hydrogen explosions are due to the high-temperature Zr oxidation. Accident-tolerant fuel (ATF) projects currently focus on applying a Cr-based metal coating to protect the Zr alloy tubing, but modifications such as alloying of Cr may be necessary to improve Cr performance.

2. Methodology

Cr-Fe and Cr-Al alloys were fabricated via vacuum arc melting followed by thermal annealing. High-temperature oxidation behaviors in static air were studied in a furnace and measuring the weight gain. Characterization of the morphology and identification of oxides formed were analyzed using SEM-EDS and GIXRD, respectively.

3. Results and Discussion

Surface delamination and spallation were observed in some specimens at 1200°C, while samples maintained the oxide scales at 1100°C. The measured weight gains are also relatively small compared to Zr alloy oxidation and comparable to pure Cr oxidation in the literature. Characterization of the oxides identified Cr_2O_3, Fe_3O_4, Fe_2O_3, and Al_2O_3 in the specimens. GIXRD results of the samples after oxidation show the distribution of oxides as function of depth.

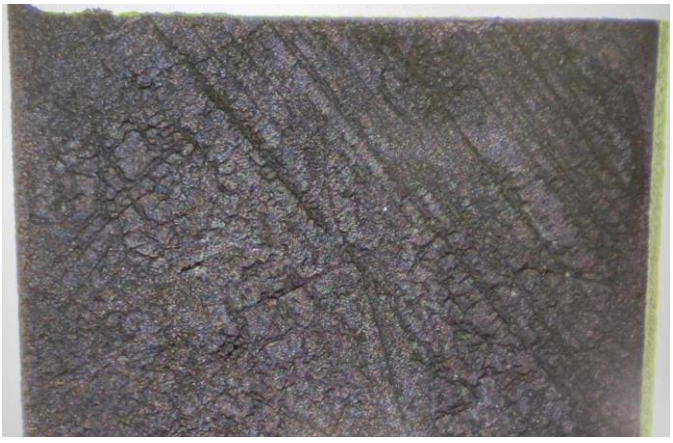

Fig 1. Cr-7Fe oxidized at 1200°C.

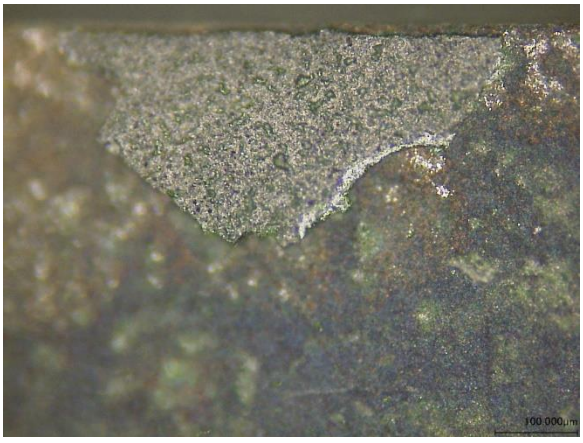

Fig 2. Cr-2Al oxidized at 1200°C

4. Conclusion

The results of high-temperature air oxidation of Cr-Fe and Cr-Al show potential improvement to pure Cr by possibly providing additional protection of the Cr_2O_3 scale for the substrate, which can be future candidates as coating. Further oxidation tests in other high-temperature atmospheres with steam are to be performed.

Evaluation of the Hoop Tensile Behavior of Cr-coated Zircaloy-4 Fuel Cladding by Advanced Expansion Due to Compression (A-EDC) Test

*Ziqi Wei[1], Bo Li[1], Lijuan Cui[3], Zongda Yang[1], Risheng Qiu[1,4], Sho Kano[2], Hiroaki Abe[1]
[1]The University of Tokyo, [2]National Institutes for Quantum Science and Technology,
[3]Sichuan University (China), [4]Chongqing University (China)

Abstract

This research evaluates the mechanical behavior and strength of Cr-coated Zircaloy-4 cladding tubes under hoop tensile stress. Cr coatings were applied to Zircaloy-4 rings using the pulsed laser deposition (PLD) method. Advanced expansion due to compression (A-EDC) tests were conducted on the as-deposited specimens at room temperature (RT) and 573K. To determine the coating's strength accurately, mechanical properties including Young's modulus and residual stress were measured using nano-indentation and XRD methods. Analyzing the crack density-local strain relationship established a quantification method for the coating's cracking behavior. The results demonstrated superior crack resistance for the thin Cr coating with a nanocrystalline/amorphous structure.

Keywords: Accident Tolerant Fuels, Cr coating, Advanced Expansion due to Compression (A-EDC) Test, Hoop strength, Crack propagation

1. Introduction

Chromium (Cr) coated zirconium-based alloy (Zry) is considered as the nearest candidate for accident-tolerant fuel (ATF) cladding materials. These coatings are likely to face axial and hoop tensile stresses, temperature variations, and other factors that can degrade the cladding and cause cracks to form on the outer layer. The Advanced Expansion-Due-to Compression (A-EDC) test, which can assess the hoop tensile mechanical properties of cladding materials, is a potential method for evaluating the hoop tensile behavior of coated cladding, particularly regarding the coating's adhesion and fracture strength.

This research qualitatively and quantitatively evaluates the mechanical behaviors of Cr-coated Zircaloy-4 cladding tubes under hoop tensile stress using the A-EDC test.

2. Experimental

Pulsed laser deposition (PLD) was used to apply Cr coatings on the outer surface of Zircaloy-4 rings. The cross-sectional structure of the as-received coatings was examined using transmission electron microscopy (TEM), with sample foils prepared via the focused ion beam (FIB) technique. Advanced Expansion-Due-to Compression (A-EDC) tests were conducted on the as-deposited specimens, using cylindrical pellets of Cu and stainless steel 316L, at RT and 573K, respectively. Young's modulus and nano-hardness were measured by nano-indentation at various indent depths. Residual stress at RT was determined using the d-sin^2(ψ) method by X-ray diffraction (XRD).

3. Results

The Cr coatings, 350 nm thick, have a bi-layer structure: a 130 nm amorphous layer and a 220 nm nano-crystalline layer. Their Young's modulus and residual stress are 227 GPa and -1.4 GPa, respectively. In A-EDC tests, transverse surface cracks perpendicular to the tensile direction and slanted cracks at a 45° angle appeared, indicating strong adhesion and strain transfer from the Zry-4 substrate. The crack density-strain relationship shows three stages: no cracking, rapid crack increase, and saturation, with slanted cracks forming after transverse ones. At 573K, the first crack forms at a strain of 0.07, higher than at RT (0.03), suggesting increased ductility due to a brittle-to-ductile transition. This implies superior fracture strength (~5.9 GPa) for the Cr coating with the nature of brittleness of Cr at RT, though determining its exact behavior remains challenging due to the unclear DBTT window for the nano-crystalline/amorphous structure.

機械学習に基づく原子力用 SiC 材料ポテンシャル関数の開発

Development of potential function for SiC materials used in nuclear applications based on machine learning

*王 抱朴[1]、祝 梁帆[1]、陳 昱婷[1]、岩切 宏友[2]、森下 和功[1]

[1]京都大学，[2]琉球大学

本研究は第一原理計算と機械学習方法を結合し、第一原理計算データを用いてニューラルネットワークを構築により、大きな適用規模と高い精度を持つ原子力用 SiC 材料のポテンシャル関数を開発した。

キーワード：SiC 材料，第一原理計算，機械学習，ポテンシャル関数，照射損傷

1. 緒言

SiC 材料は多くの点で優れた特性を持っており、原子力材料として開発と検証が進められている。原子炉内の環境が材料に及ぼす影響を研究するため、分子動力学法を用いて材料の照射損傷挙動を分析できる。分子動力学法の信頼性は使用される原子間ポテンシャル関数の精度に依存している。しかし、現在 SiC 材料の分子動力学シミュレーションに広く用いられている Tersoff と MEAM ポテンシャル関数は、欠陥形成エネルギーの第一原理計算結果と一致しないことが確認されている。GW−ZBL ポテンシャルはより正確な欠陥形成エネルギーを提供することができるが、欠陥移動エネルギー障壁の計算に対する信頼性は低い[1]。これらのポテンシャル関数を用いて SiC の照射損傷挙動シミュレーションを行うと、研究の信頼性が低下する可能性がある。そのため、原子間相互作用を正確に記述できる新たなポテンシャル関数の開発が求められている。第一原理計算は量子力学の基本原理に基づく計算方法により、より正確な原子間ポテンシャルを得ることができるが、その系は数百原子に限られ、計算コストが高く、適用規模は小さいである。一方、人工知能技術の発展に伴い、機械学習方法が第一原理計算で得られるデータを学習し、ニューラルネットワークポテンシャル関数を構築することは、計算速度と規模を向上させることができる。そこで、照射損傷挙動に対して信頼性の高い分子動力学シミュレーションを行うために、本研究では、高精度とされる第一原理計算方法を用いて、SiC のポテンシャルエネルギーを計算し、ニューラルネットワークを構築し、大きな適用規模と高い精度を兼ね備える SiC のポテンシャル関数を開発した。

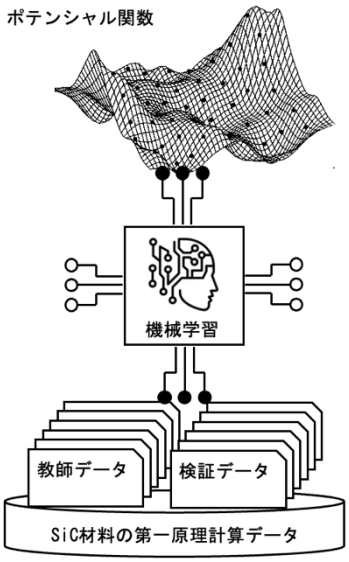

図 1　第一原理計算と機械学習の結合

2. 計算

第一原理計算は SIESTA コードを用いて QST のスーパーコンピュータで行った。ニューラルネットワークの構築は dpdata や DeePMD-kit などのコードを使用した。ポテンシャル関数に良好な汎化能力を持たせるために、完全結晶構造、異なる格子定数、および空孔や格子間原子が存在する構造で計算と訓練を行った。

3. 結果

216 原子を含む、合計 149 構造の SiC の第一原理計算スーパーセルを構築した。図 2 に示すディープニューラルネットワークを開発し、隠れ層はポテンシャル関数として抽出された。

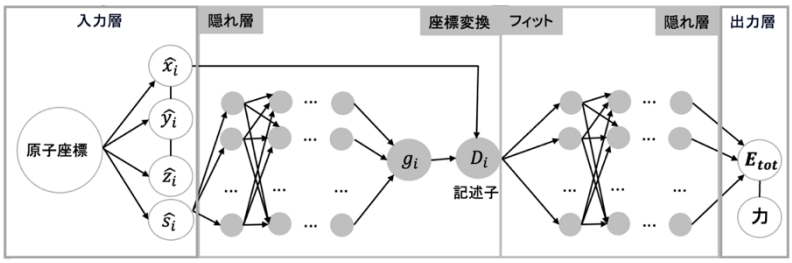

図 2　開発されたディープニューラルネットワーク（DNN）

参考文献

[1] G. D. Samolyuk, et al. Journal of Nuclear Materials, 2015, 465 (83-88).

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*Baopu Wang[1], Liangfan Zhu[1], Yuting Cheng[1], Hirotomo Iwakiri[2] and Kazunori Morishita[1]

[1]Kyoto Univ., [2]Ryukyus Univ.