## A HYBRID EXPERIMENTAL AND NUMERICAL INVESTIGATION ON THE FRACTURE PROPERTIES OF ZIRCONIUM WITH MAX PHASE COATINGS COVERING A WIDE RANGE OF STRESS STATES

Boyu Pan<sup>1\*</sup>, Fuhui Shen<sup>1</sup>, Markus Könemann<sup>1</sup>, Matej Fekete<sup>2</sup>, Sebastian Münstermann<sup>1</sup>,

Jochen M. Schneider<sup>2</sup>

<sup>1</sup>Integrity of Materials and Structures, Steel Institute, RWTH Aachen University, Intzestraße 1, Aachen 52072, Germany

<sup>2</sup>Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, Aachen D-52074, Germany \* Presenting Author email: boyu.pan@iehk.rwth-aachen.de

#### Abstract

This work aims to carry out a hybrid experimental and numerical investigation on the fracture properties of the zirconium cladding tube coated with Cr<sub>2</sub>AlC, which belongs to the group of MAX phase materials. A macroscopic failure criterion is finally developed based on the experimental and numerical simulation results, thus contributing to the design of the accident-tolerant fuel system (ATFs) in nuclear power plants. A series of in-situ bending tests involving various sample geometries covering a wide range of stress states are carried out under a quasi-static condition. Oxidized samples and samples aged in hot water under high pressure are also involved to consider the aging and oxidation effect on material failure. The modified Bai-Wierzbicki (MBW) damage model and the analytical Yoon2014 model are coupled in the simulation so the damage and strength differential effect can be considered in modeling material failure. By transferring boundary conditions between the micro- and macroscopic model as a weak macro-micro coupling, homogenization is achieved so that a micromechanical sub-model can also be developed and the micromechanical simulation and macroscopic simulation can be cross-scale bridged.

## 1. Introduction

Following the Fukushima reactor accident, concepts and materials systems are being developed around the world to improve reactor safety, among which the development of accident-tolerant fuel systems (ATFs) particularly concerning cladding concepts is one of the many focuses. The systems to be developed should overcome the current technical limitations of conventional zirconium cladding tube systems and thus contribute to a significant extension of service life, especially under accident conditions. This paper proposed a macroscopic failure criterion based on the in-situ bending tests and numerical simulation results of the zirconium cladding tube coated with Cr<sub>2</sub>AlC. Cr<sub>2</sub>AlC belongs to the group of MAX phase materials and it features high thermal shock resistance and good corrosion resistance. Samples of various geometries are involved in the test to cover a wide range of stress states; in addition, oxidized samples and samples aged in hot water under high pressure are tested to consider the aging/oxidation effect on material failure. Furthermore, by transferring boundary conditions between the micro- and macroscopic model as a weak macro-micro coupling, homogenization is achieved so that a micromechanical sub-model can also be developed and the micromechanical simulation and macroscopic simulation can be cross-scale bridged.

#### 2. Results

The general methodological flow of the study is illustrated in Figure 1. It starts from the characterization of basic mechanical properties of the zirconium substrate and Cr<sub>2</sub>AlC, and it bridges the mechanical performance with mechanical properties via a hybrid experimental and numerical method. Various sample geometries covering a wide range of stress states are carried out under a quasi-static condition. Oxidized samples and samples aged in hot water under high pressure are also involved to consider the aging and oxidation effect on material failure. The modified Bai-Wierzbicki (MBW) damage model [1] and the analytical Yoon2014 model [2] are coupled in the simulation so the damage and strength differential effect can be considered in modeling material failure. With the aid of the proposed macroscopic failure criterion, the design of ATFs can be evaluated and optimized in the future. Furthermore, by transferring boundary conditions between the micro- and macroscopic model as a weak macro-micro coupling, homogenization



is achieved so that a micromechanical sub-model can also be developed and the micromechanical simulation and macroscopic simulation can be cross-scale bridged.

Figure 1. Methodological flow of the hybrid experimental and numerical study on the zirconium cladding tube coated with Cr<sub>2</sub>AlC.

# 3. Conclusions

This study identifies the hardening and fracture properties of the zirconium cladding tube coated with  $Cr_2AlC$  belonging to the MAX phase material by carrying out in-situ bending tests involving samples of various geometries and under various processing methods. A macroscopic failure criterion is developed, with which the design of this ATFs can be evaluated and improved.

# Acknowledgments

The authors gratefully acknowledge the Society for Plant and Reactor Safety (GRS) [grant number: 100513703] for the financial funding for the project.

# References

[1] Lian, J., Sharaf, M., Archie, F., & Münstermann, S. (2013). A hybrid approach for modelling of plasticity and failure behaviour of advanced high-strength steel sheets. *International Journal of Damage Mechanics*, 22(2), 188-218.

[2] Hu, Q., & Yoon, J. W. (2021). Analytical description of an asymmetric yield function (Yoon2014) by considering anisotropic hardening under non-associated flow rule. *International Journal of Plasticity*, 140, 102978