Coupled modelling of ZrO$_2$ / α-Zr(O) layers growth under thermal and mechanical gradients

Jean-Baptiste Minne[*,†], Virgil Optasanu[†] and Tony Montesin[†]

[†] ICB UMR 6303 CNRS – Université de Bourgogne,
9 Av Alain Savary 21078 Dijon Cedex France
e-mail: jean-baptiste.minne@u-bourgogne.fr , virgil.optasanu@u-bourgogne.fr,
tony.montesin@u-bourgogne.fr - web page: http://icb.u-bourgogne.fr

ABSTRACT

The oxidation process of a nuclear reactor fuel rod clad made of zirconium is simulated. It is assumed that oxygen is transported by anionic diffusion in the zirconia layer (ZrO$_2$), reacts at the interface between the zirconia layer and the metal and diffuses in the oxygen-enriched metal volume (α-Zr(O)) by an interstitial mechanism. The model is based on the thermodynamics of irreversible processes and takes into account the influence of driving forces on the oxygen migration in the metal such as the oxygen concentration gradient, the temperature gradient [1] and the mechanical stress gradient [2]. The growth of both ZrO$_2$ and α-Zr(O) layers are simulated using the finite element software CAST3M.

This model has been applied on an axisymmetric geometry by imposing a heat flow on the fuel side and a constant temperature on the waterside of the clad. Depending on the value of some coupling parameters, part of them remaining still unevaluated for oxygen in zirconium, results are related to differences in oxidation kinetics and oxygen distributions observed on the inner and outer side of nuclear clads. Thus, we show that negative values for the heat of transport, which relies the gradient of concentration and the gradient of temperature, give coherent results with experimental observations on oxidation kinetics for both sides of the clad.

REFERENCES

[1] G. D. Rieck, D. L. Vogel, Thermotransport of oxygen in β-zirconium, Acta Metallurgica, vol. 14, pp. 1703-1714, 1966

[2] Jean-Baptiste Minne, 2013, Contribution à la modélisation du couplage mécanique/chimique de l'évolution de l'interface pastille-gaine sous irradiation, PhD Thesis, Université de Bourgogne