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FINITE ELEMENT MODELING OF ZIRCONIUM-BASED ALLOYS OXIDATION

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In Pressurized Water Reactor (PWR), zirconium-based alloy cladding tubes are immersed in a corrosive environment: high pressure water at high temperature with boron and lithium. The fuel cladding corrosion, specially the oxidation of the zirconium alloy, is one of the main factors limiting the in-pile fuel rods service time (~ 5 years). Therefore it is important to predict the corrosion process of zirconium-based alloys in PWR conditions. The aim of this work is to implement the diffusion-corrosion phenomenon in a standard finite element code (Cast3M, developed at CEA) in order to simulate the oxidation kinetics observed in pre-transient phase of the Zr alloys.

Indeed many experimental results indicate that the zirconium oxidation kinetic does not follow the predicted parabolic law from Wagner's theory. Oxidation experiments show that the kinetic have rather a sub-parabolic or cubic behavior. This gap between theory and experiment could be partly explained by the evolution of the stress and its gradient existing in the oxide scale. In order to simulate the sub-parabolic kinetic, our numerical model takes into account the stress influence on oxygen diffusion flux, as well as the modification of the grain size of the oxide during the pre-transition stage.

In Finite Element calculation, the main difficulty is the modeling of metal/oxide interface. Indeed, the oxygen concentration profile has a discontinuity at the internal interface due to sharp variations of oxygen concentration and diffusive properties between the two phases. This mobile discontinuity is difficult to implement with the standard Finite Element Method. First, we developed a diffuse interface 1D-model taking inspiration from phase field model [1]. In a phase field model, the zero thickness interface is replaced by a volume in which properties are homogenized with the volume fraction of the two phases. This is called the "mixing zone". Thus, changing from one material to another does not present properties discontinuity. But this first model leads to a too thick mixing zone that modifies the oxidation kinetics depending on the properties of the mixing zone. For this reason, we developed a

second model to limit the thickness of the mixing zone to a single finite element in order to be closer to the physical process. Thus we get a moving mixing zone reduced to one element (in the range of several nanometers) and so, a moving metal/oxide interface determining the oxide thickness. The two approaches will be compared to the results of corrosion tests performed in autoclave.

REFERENCES

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