



Cladding oxidation model development based on diffusion equations and a simulation of the monoclinic-tetragonal phase transformation of zirconia during transient oxidation



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ARTICLE INFO

Article history:

Received 10 September 2013

Accepted 19 March 2014

Available online 27 March 2014

ABSTRACT

Zircaloy cladding oxidation is mostly represented by parabolic rate correlation. But the correlation approach is not suitable for long-term isothermal oxidation [4] or oxidation occurs under steam starvation conditions [5] and cannot obtain the detailed oxygen distribution which impacts the detailed mechanical behavior. To obtain the detailed oxygen distribution, a multi-phase diffusion problem with moving boundaries was introduced to simulate the cladding oxidation [9,10]. However, the hysteresis phenomenon related to the coexistence of monoclinic-tetragonal phases of zirconia which are very important to model the cladding oxidation during a LOCA, is not analyzed. In this study, a cladding oxidation model based on diffusion equations in the temperature range from 923 K to 2098 K which contains β -Zr, α -Zr, monoclinic-ZrO₂, tetragonal-ZrO₂, and cubic-ZrO₂ is developed and the detailed oxygen distribution in the cladding could be obtained. It showed that the simulations of short-term and long-term isothermal oxidation, transient oxidation, and oxidation under steam starvation conditions were reasonable through comparing with the experimental data. We found that our model can give a reasonable simulation of the hysteresis phenomenon of monoclinic-tetragonal phase transformation during transient oxidation as well as a much better simulation of the hypothetical LOCA transient oxidation experiments [11] in ORNL than that by the code based on the parabolic rate correlation. This indicates that the developed model can accurately simulate the cladding oxidation during a LOCA transient.

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1. Introduction

Cladding oxidation is important during a loss-of-coolant accident (LOCA) or a severe accident. It has great impact on the detailed mechanical behavior of the cladding. When the emergency core cooling water is injected to reflood the hot core during a LOCA or at the early phase of a severe accident, the cladding will undergo a thermal shrinkage. If the embrittled cladding cannot stand the stress, the cladding will crack, which results in massive hydrogen formation and additional heat production, and a release of radioactive fission product.

In many severe accident analysis codes [1–3], cladding oxidation is represented by parabolic rate correlations, such as Urbanic–Heidrick, Prater–Courtright, and Cathcart–Pawel correlation. However, the correlation approach is not suitable for long-term

isothermal oxidation [4] or oxidation occurs under steam starvation conditions [5]. In addition, using this approach, it is not possible to obtain detailed oxygen distribution in the cladding which has great impact on the detailed mechanical behavior, such as the shattering of cladding. For example, because SCDAP/RELAP5 uses parabolic rate equations to define oxidation, and does not calculate the profile of oxygen distribution through the cladding, the proposed shattering criterion deviates from the experiment of Chung and Kassner [6] when the maximum cladding temperature exceeds 1560 K, and the enhanced oxidation during reflooding phase will be under-predicted. Actually, a conclusion can be made according to the studies of Pawel, Sawatzky, Chung-Kassner, Jun Hwan Kim [7,8]: the shattering of cladding is related to the distribution of oxygen concentration in the cladding. Hence, it is necessary to develop a cladding oxidation model to obtain the distribution of oxygen concentration in the cladding.

To obtain the distribution of oxygen concentration in the cladding, a multi-phase diffusion problem with moving boundaries was also introduced to simulate the cladding oxidation in a previous study [9]. Recently, Berdyshev and Veshchunov [10]

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Nomenclature

$C_{x/y}$	equilibrium oxygen concentrations in the x phase at the x/y interface
c_i	oxygen molar density of phase i at time t and distance r from the cladding axis
$c_i^{(1)}$	oxygen molar density at the left boundaries of phase i correspondingly
$c_i^{(2)}$	oxygen molar density at the right boundaries of phase i correspondingly
$c_{i, \text{equilibrium}}^{(1)}$	the equilibrium oxygen concentration at the left boundary of phase i
$c_{i, \text{equilibrium}}^{(2)}$	the equilibrium oxygen concentration at the right boundary of phase i
D_i	diffusion coefficient of oxygen in phase i
F_i	the oxygen flux
K_{ox}	parabolic coefficient related to the oxide layer
K_{α}	parabolic coefficient related to the α -Zr layer
K_w	parabolic coefficient related to the mass of oxygen absorbed
l_{ox}	the thickness of the oxide layer
l_{α}	the thickness of the α -Zr layer
Q_0	the oxygen flux at the inner face of the cladding
Q_3	the oxygen flux at the external face of the cladding
R_{inside}	the coordinate of inside of the cladding before oxidation

R_{outside}	the coordinate of outside of the cladding before oxidation
v_i	the convective velocity of phase i
w_o	the mass of oxygen absorbed by cladding per unit area

Greek symbols

ΔR	thickness of the cladding before oxidation
ρ_i	the zirconium or zirconia molar density
τ_i	the characteristic relaxation time in phase i
ξ_i	the interface coordinate between phase i and $i - 1$ in coordinate r
Ψ_i	the interface coordinate between phase i and $i - 1$ in coordinate x

Subscript

cu	cubic-ZrO ₂
mo	monoclinic-ZrO ₂
ox	all phases of ZrO ₂
st	steam
te	tetragonal-ZrO ₂
α	α -Zr
β	β -Zr

developed a model for high-temperature oxidation of Zr cladding in steam under fast transient conditions. However, this model did not take the low temperatures (below 1273 K) conditions into account. Therefore, the oxygen diffusion coefficient in ZrO₂ (monoclinic) phase could not be obtained and it was not possible to analyze the phenomena (especially the hysteresis phenomenon) related to the coexistence of monoclinic and tetragonal phases which are very important to model the cladding oxidation during a LOCA. For example, in ORNL, the oxide layer thicknesses of three hypothetical LOCA transient tests are more than 100% over-estimated by the code based on the parabolic rate correlation of the tetragonal phase [11]. The reason is related to the hysteresis phenomenon of monoclinic-tetragonal phase transformation. Fig. 1 illustrates this phenomenon [12]. It can be inferred that the transformation occurs during heating around 1473 K, while the inverse transformation during cooling occurs below 1273 K. In order to simulate the cladding oxidation accurately, it is necessary to analyze the monoclinic-tetragonal phase transformation of zirconia.

The objective of this study is to develop a cladding oxidation model to predict zircaloy cladding oxidation at typical conditions (short-term, long-term isothermal oxidation, transient oxidation, and oxidation under steam starvation conditions), and the phenomena related to mechanical stresses, such as breakaway phenomenon are not considered. The model is applicable from 923 K to 2098 K which contains β -Zr, α -Zr, monoclinic-ZrO₂, tetragonal-ZrO₂, and cubic-ZrO₂. Based on this model, the hysteresis phenomenon related to the coexistence of monoclinic-tetragonal phases of zirconia can be analyzed.

2. Cladding oxidation model

The cladding material is zircaloy-4 in the oxidation model development. The impacts of irradiation, hydrogen and pressure on cladding oxidation are neglected in the present model. Temperature range is from 923 K to 2098 K.

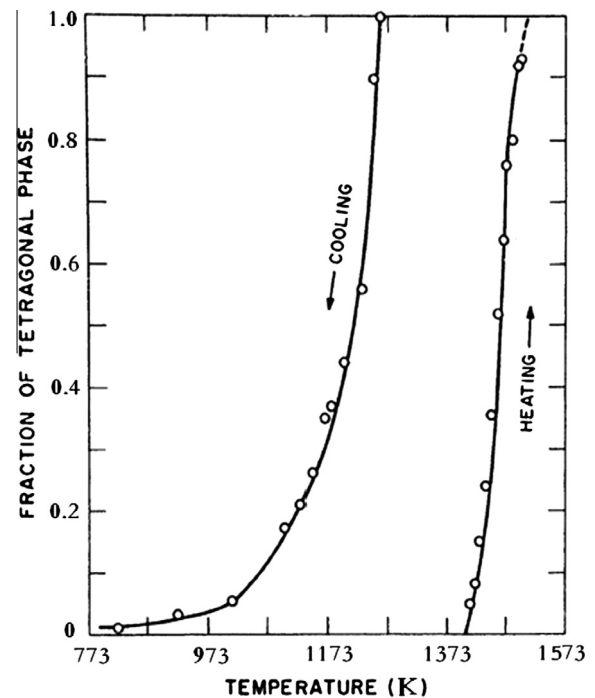


Fig. 1. Hysteresis phenomenon in the monoclinic-tetragonal phase transformation in ZrO₂ [12].

2.1. Basic equations

The present cladding oxidation model is a one-dimension model. Oxidation in the cladding is assumed axis-symmetrical, that is, oxidation is the same along the circumferential direction. Another assumption is that oxidation in one axis position has no impact on other axis positions. Therefore, diffusion of oxygen atoms can only occur in the radial direction.

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