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Theoretical Modeling of Protective Oxide Layer Growth in Non-isothermal Lead-Alloys Coolant Systems: Quarterly Progress Report (01/01/06- 03/31/06)

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Task 21: Theoretical Modeling of Protective Oxide Layer Growth in Non-isothermal Lead-Alloys Coolant Systems

Quarterly Progress Report
01/01/06- 03/31/06

UNLV-TRP University Participation Program

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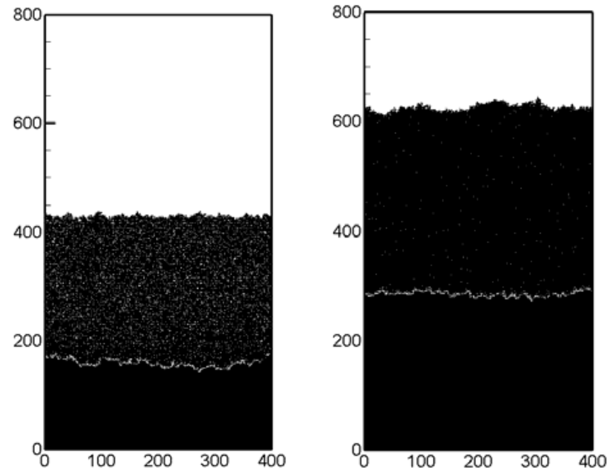
Research highlights

- A cellular automaton model using method of global restructuring on the growth and corrosion during the formation of the passive layer has been developed.
- A stochastic model, which combines the surface growth and internal oxidation, has been developed to explain the oxidation mechanism of steels in liquid lead-alloys.
- Two conference papers have been accepted and will be presented in 2006 International Congress on the Advances in Nuclear Power Plants (ICAPP '06).

Technical progress report

(1) Global restructuring cellular automaton model on growth and corrosion behavior during the formation of passive layer

The corrosion induces a restructuring in the layer, which will induce porosity in the part of the oxidation layer. Figure 1 shows the snapshots of the simulated layer with the presence of corrosion. For different control parameters, the layer exhibits for different porosity. Figure 2 shows the height of the growth front and the global porosity in the case with corrosion as a function of time steps. As shown in the figure, the slope of the corresponding straight line is about 0.5, which approximates the growth front as the square root of time. Hence, this model can be interpreted by the Wagner theory, and the parabolic law is suitable for this case.



(a) $n = 1$ (b) $n = 2$

Figure 1. Snapshots of the simulated layer in the presence of corrosion. They correspond to 10^5 time step. The black dots are either metal or oxide sites. The white spaces are occupied by either solvent or corrosion sites. The initial interface between metal and solvent locates at $j = 400$. n represents the number of entity of metal particles which locates on single metal site.

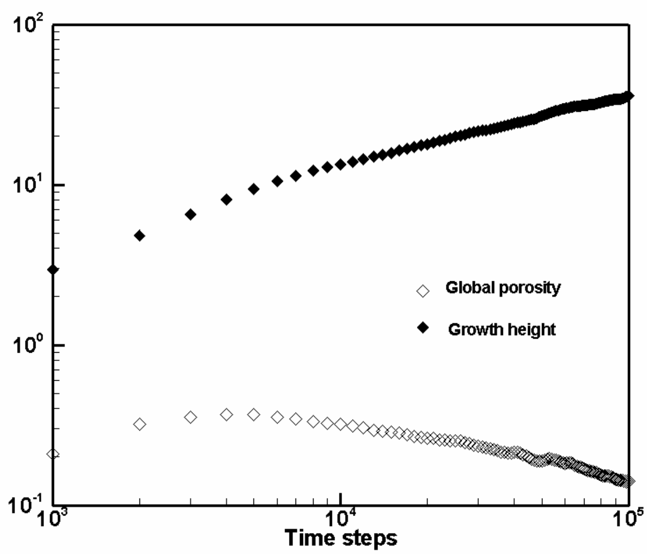
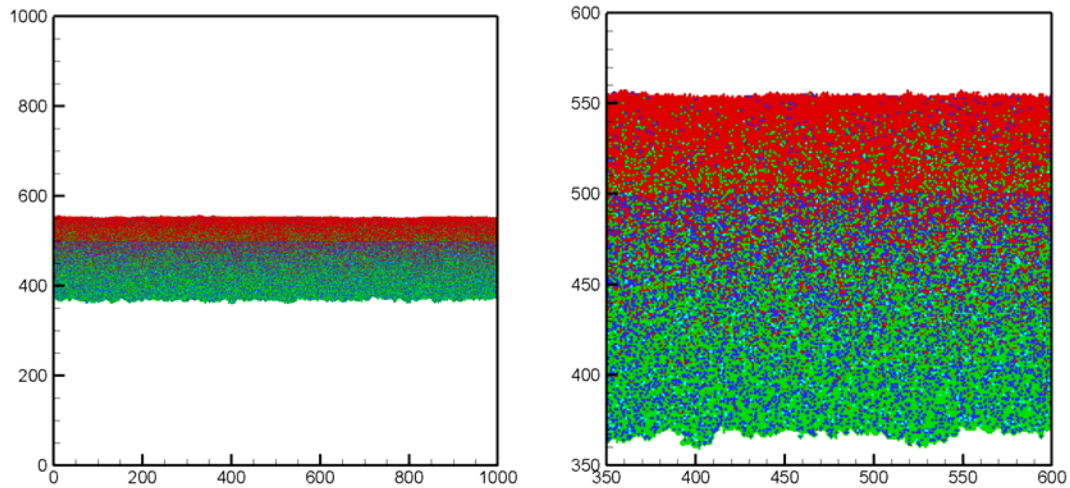


Figure 2. Global porosity and dimensionless growth height for the case with corrosion as a function of time steps. The growth height is normalized by spatial difference.

(2) Stochastic modeling on the surface growth and internal oxidation

In this model, three main processes, which include the corrosion of the substrate, the diffusion of iron species across the oxide layer and precipitation of iron on the oxide layer, are simulated. The diffusion process is modeled by the Kawasaki random walk model. This model also includes the effect of volume expansion on the oxide layer growth during oxidation. Figure 3 shows the snapshots of simulated duplex layer with presence of corrosion and precipitation. As seen in Figure 3, the duplex oxide layer can

be found in this model. The structure of oxide layer coincides with Robertson theory, and the oxide growth mainly is controlled by the outward diffusion of iron. Figure 4 shows the variation of growth/corrosion front as a function of time step. Since the mechanism of the process of formation of oxide layer is controlled by diffusion of A and B, parabolic growth rate is suitable for both growth fronts and corrosive front.



(a) Full view (b) Zoom view

Figure 3. Snapshots of the simulated layer in the presence of corrosion and surface growth. They correspond to 10^4 time step. The red dot is Fe_3O_4 site; the blue dot is Cr site; the green dot is Fe site; the cyan dot is Cr_2O_3 site. Upper side of layer is filled with liquid LBE with low oxygen concentration. Lower side of the oxide layer is steel. The corrosion probabilities of Fe and Cr are taken as 0.5.

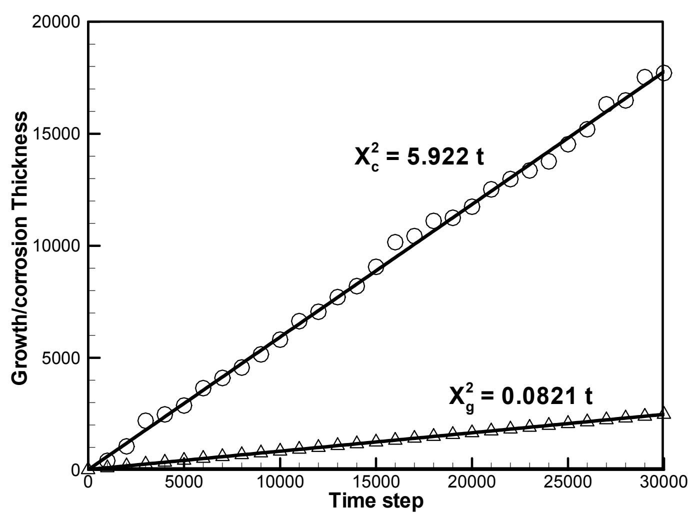


Figure 4. Variation of growth/corrosion front as a function of time step. The curve with symbol circle is the growth front and the curve with symbol triangle is the corrosion front.

(3) Two conference papers have been accepted and will be presented in 2006 International Congress on the Advances in Nuclear Power Plants (ICAPP '06)

1. Huajun Chen, Yitung Chen, Jinsuo Zhang, Modeling on Oxygen Transfer in the Forced Convection Lead-bismuth Eutectic Flow, ICAPP'06.
2. Taide Tan, Huajun Chen, Yitung Chen, Xianfang Tan, Hsuan-Tsung Hsieh, Analytical Modeling and Numerical Simulation of the Corrosion and Precipitation in Non-isothermal LBE Pipe/Loop Systems, ICAPP'06.