Cellular Automaton for Simulation of Oxide Layer Growth Influenced by Chromium Concentration of Structure Material

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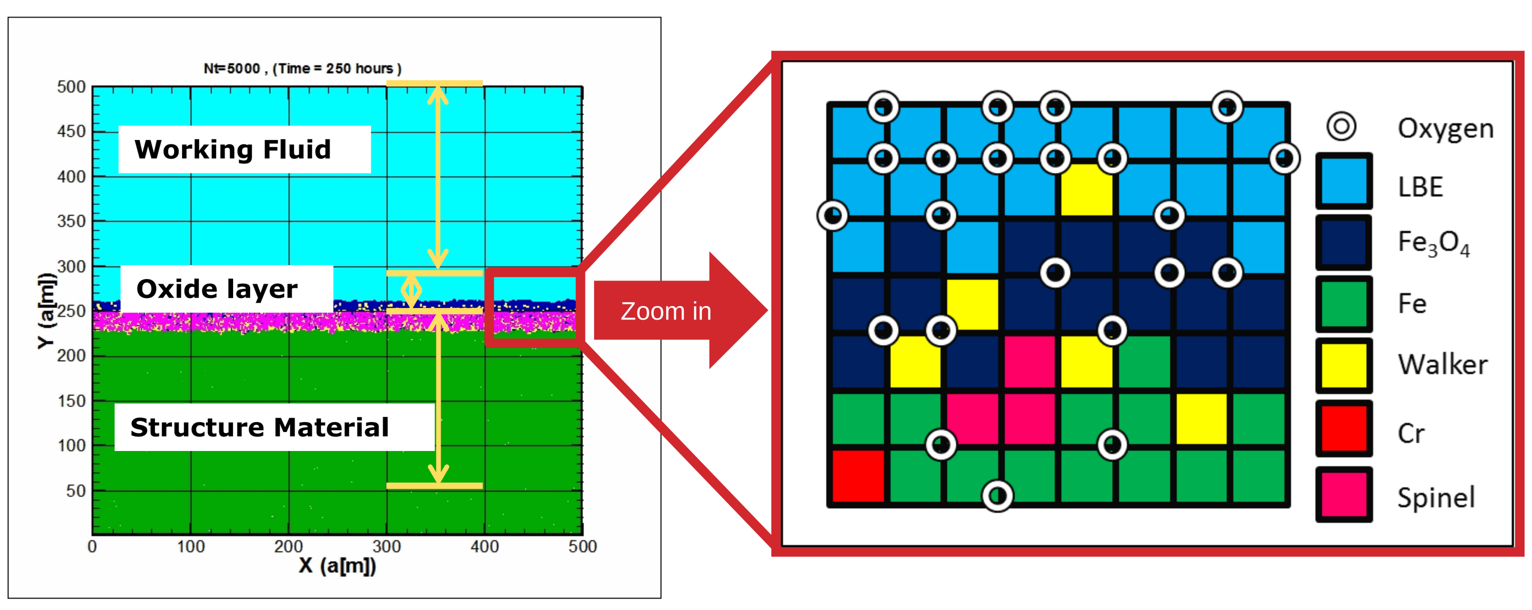
ABSTRACT

Chromium, an important alloying element, has been added in ferrous and nickel based alloy such as stainless steels and Inconel alloy to improve the corrosion resistance. High corrosion resistance of structural materials in extremely high working temperature is one crucial R&D objective of Gen IV nuclear power plants which propose to raise the thermal efficiency via high working temperature. A cellular automaton (CA) model based on the stochastic approach was proposed to simulate the process of oxidation and corrosion of structural material in flowing fluid. The relation of chromium concentration against oxide layer thickness during a specific period was found. The material containing a specific amount of chromium content shows the thinnest oxide layer on its surface, which shows the strongest ability of corrosion resistance The result of simulation is close to that of experiments, which demonstrates that the CA model will have potential to achieve the goal of this kind of study. Moreover, it not only brings the benefit to save considerably experimental time and resources but also helps researchers to find out the optimized chromium content for the best corrosion resistance.

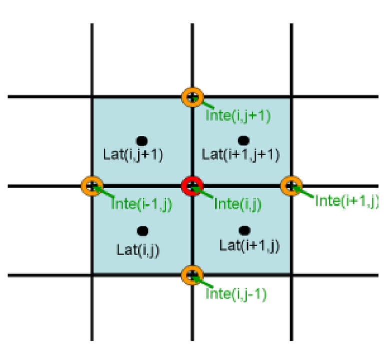
Cellular Automaton Model

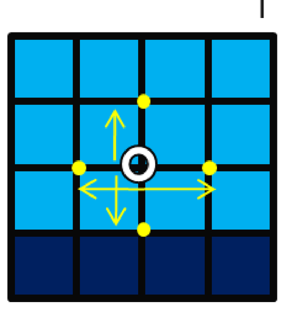
Cross section and Zoom-in view of CA model



Modified Moore Neighborhood Model

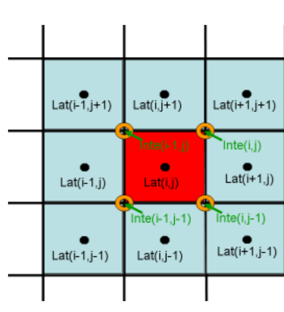
4 interstitial sites
(in boundary of lattice)

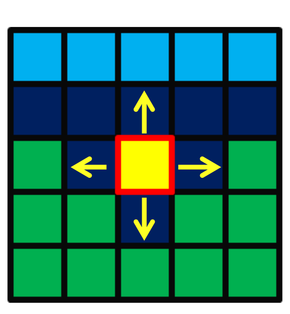




- Oxygen will move along with interstitial sites.

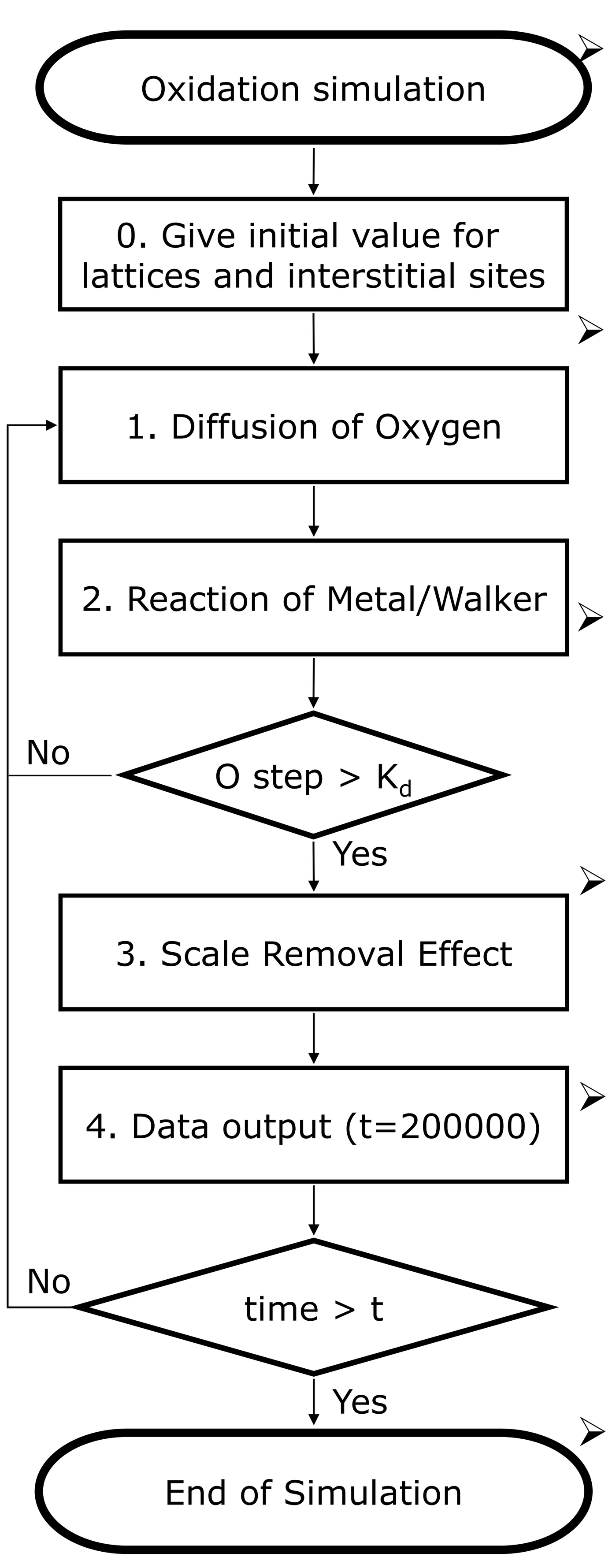
8 neighbor lattices
(in lattice)





- Species will move along with lattice sites when it matches the condition of reaction.

Working Flow of CA model

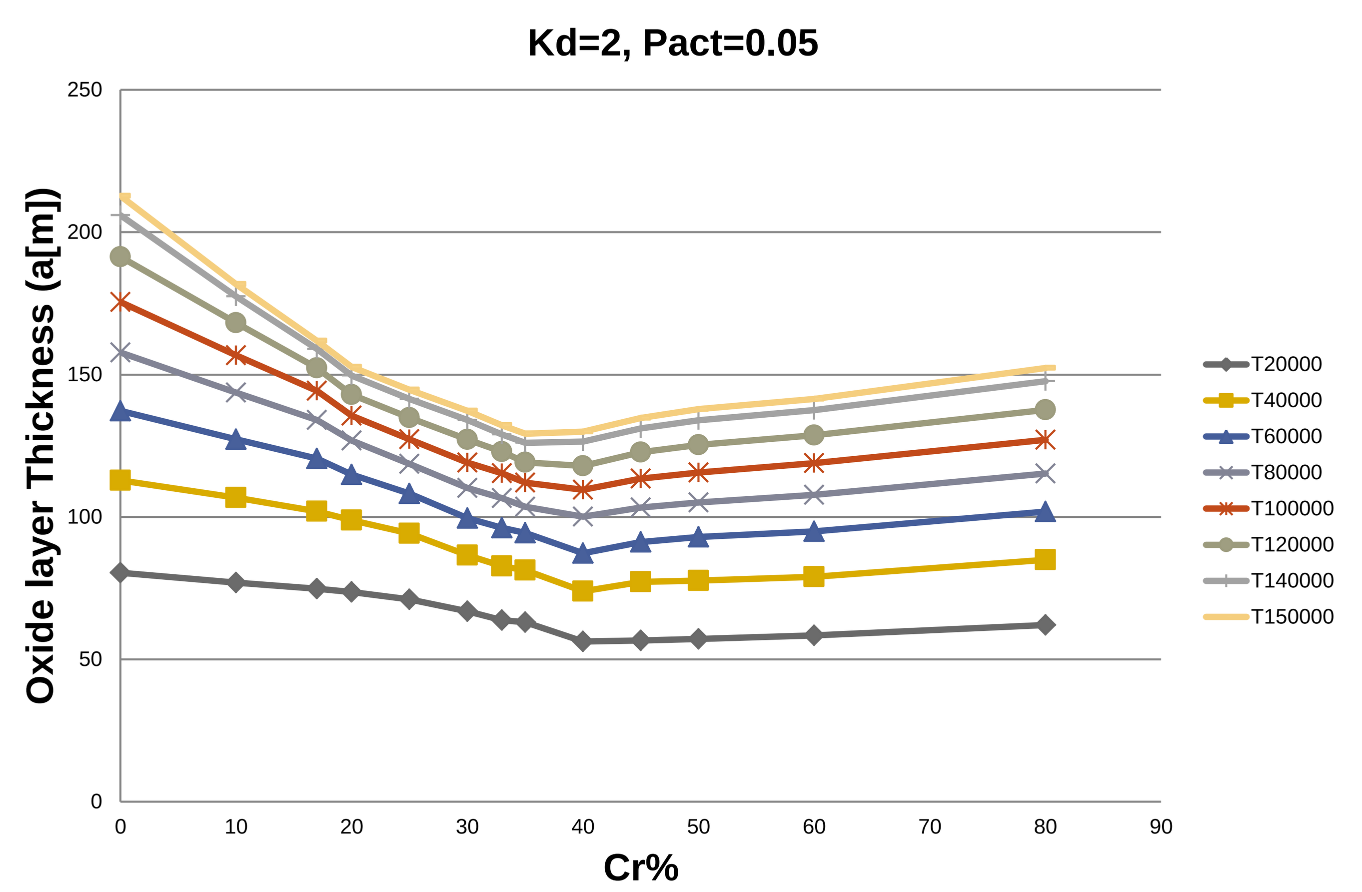


- 0. Initial value: a site which will be occupied by metal or oxide in solid phase/LBE in liquid phase.
- 1. The atomic oxygen transports randomly in four possible directions along the interstitial edge of the lattices in the oxide layer or the metal zone.
- 2. Oxidation and ionization at the inner interface of oxide/metal or at the outer surface of oxide/LBE will happen
- $$K_d = \frac{\text{Diffusion rate of oxygen}}{\text{Diffusion rate of ion}}$$
- 3. The flow direction of LBE is assumed from left to right. The morphology and roughness of the oxide/flow interface do influence on scale removal effect.
- 4. Output all results including thickness of oxide layer, concentration and coordinate of each element.

Results and Discussions

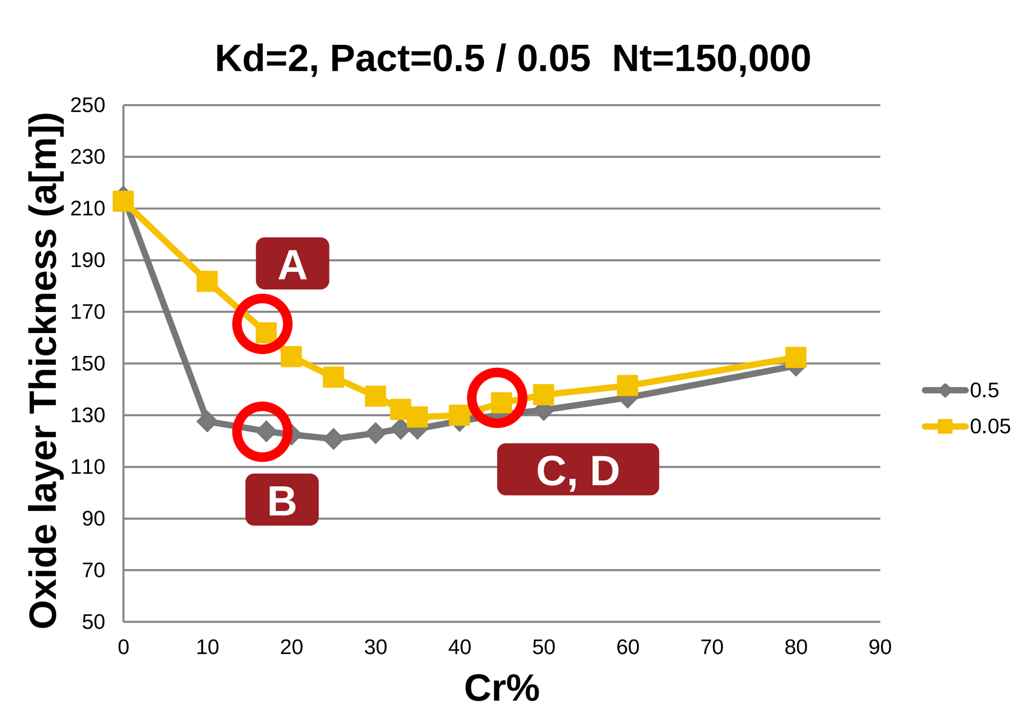
- The material with the thinnest oxide layer thickness represents the best corrosion resistance. Relations of oxide layer thickness and chromium concentration are displayed as following:

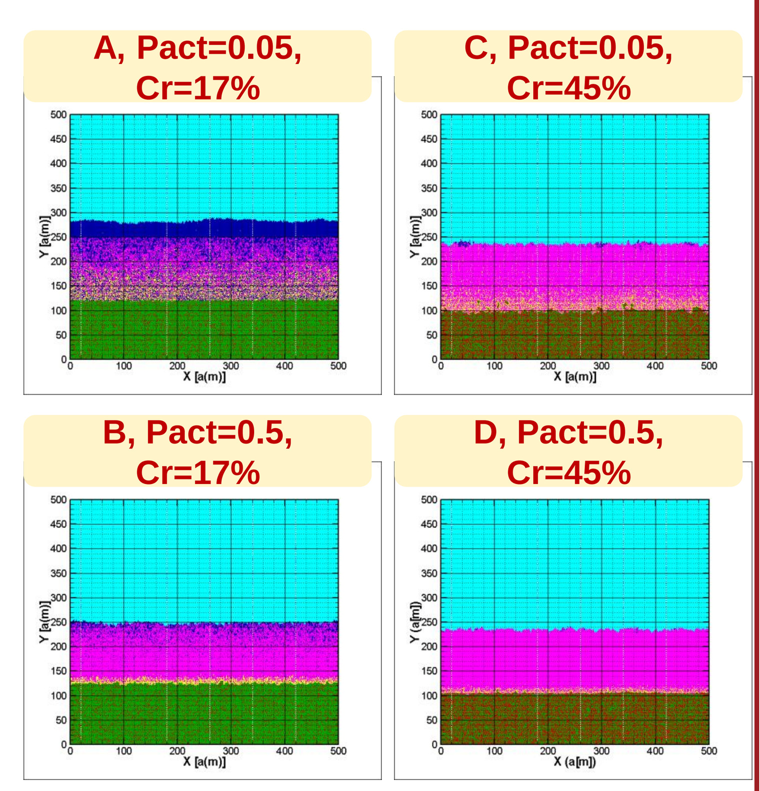
Effect of Time



- K_d means ratio of transportation rate between oxygen and metal ion (Fe^{2+}), and P_{act} signifies the reaction probability.
- As K_d=2 and P_{act}=0.05, the compositions with thinnest oxide layer corrosion resistance changes with simulation steps. The optimized composition of structure material to achieve the highest corrosion resistance are different considering its operating time.

Effect of P_{act}





- As K_d=2, N_t=150,000, the results with P_{act}=0.5 shows a better corrosion resistance than those with P_{act}=0.05
- P_{act} ↑
  - ➔Probability of oxidation ↑
  - ➔Early formation of the layer of compact Fe-Cr spinel
  - ➔For longer period, growth rate of oxide layer↓
  - ➔Better corrosion resistance
- Cr% higher than 35%
  - ➔ Concentration of chromium promise a compact enough of spinel layer
  - ➔Ability of inhibition the growth of oxide layer as P_{act}=0.05 is similar to that as P_{act}=0.5

SUMMARY

- The optimized composition of structure material to achieve the highest corrosion resistance in LBE fluid are different considering its operating time
- Variation of reaction probability P_{act} will lead to the change of oxide layer. Higher P_{act} yield a thinner and denser oxide layer, which represents a higher corrosion resistance. High P_{act} can also provide a lower Cr% (=25%) with the thinnest oxide layer as simulating time steps =150,000.
- This Cellular Automaton Model shows a potential to help researchers save more time and cost on finding out the optimized composition of structure materials.