Chemical ordering effect on the radiation resistance of a CoNiCrFeMn high-entropy alloy

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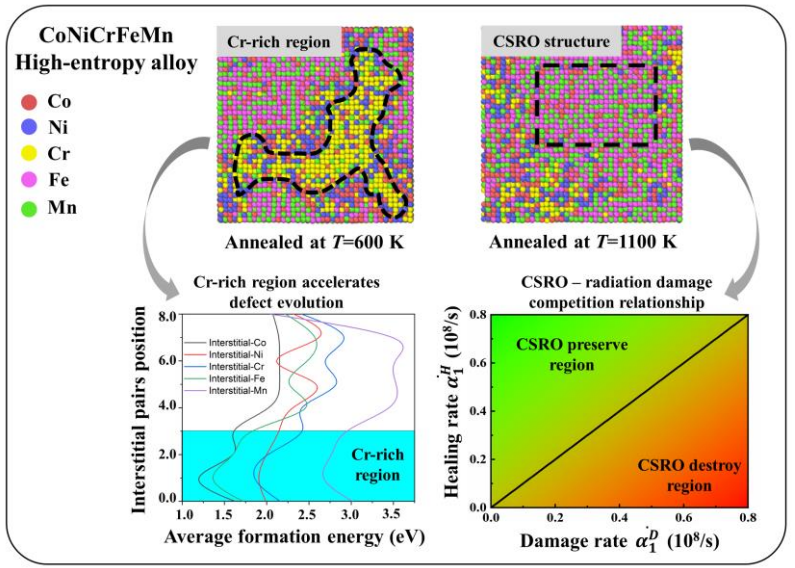
Purpose: To design better radiation resistance materials for the next-generation nuclear reactor.

Outline: Chemical ordering and its effect on the radiation resistance of CoNiCrFeMn high-entropy alloy.

Results: By using Monte-Carlo and Molecular dynamics simulations, we found that the annealing temperature of the alloys, which leads to temperature dependent chemical ordering, strongly influences the radiation resistance of CoNiCrFeMn at low dpa radiation. Annealing at 600 K, phase decomposition led to the formation of an initial stage Cr-rich region and reduced the radiation resistance. Annealing at 1100K, a chemical short-range order (CSRO) structure was formed, leading to a delay of defect number growth and dislocation density decrease. In addition, we proposed a CSRO radiation damage – diffusion healing competition model, which demonstrates that the CSRO and the key anti-damage mechanisms can be maintained at the working temperature of 1100K under a relatively lower damage rate.



Computing system: **Octopus**

- **node-hour:** 1000 node-hour
- **memory used:** 50 GB
- **vector per:** 85 %
- **parallelize:** 2-4 nodes