Atomistic simulation of interstitial and vacancy diffusivity by chemical ordering control in CrCoNi

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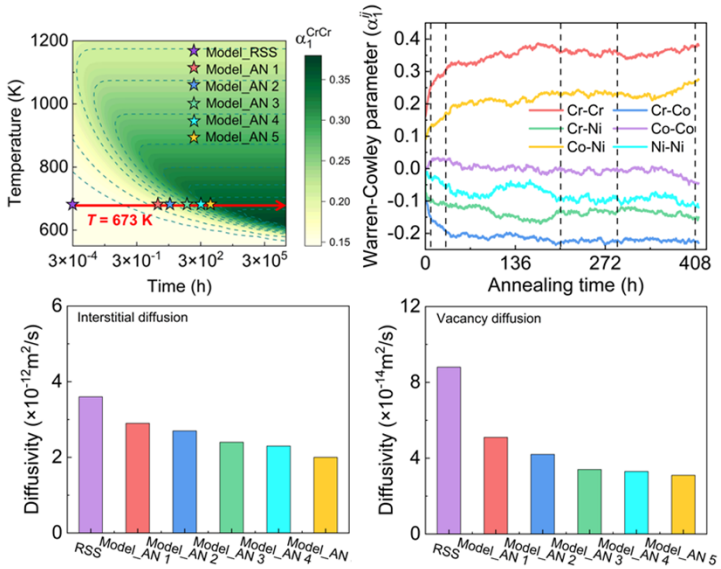
Purpose To investigate the chemical ordering formation and its effect on interstitial and vacancy diffusion in CrCoNi.
Outline Chemical ordering impact on interstitial and vacancy diffusion in CrCoNi using atomistic simulation.
Result In this work, we explored the influence of chemical ordering on interstitial and vacancy diffusion in CrCoNi MEA, illustrating the potential to modulate this diffusivity by adjusting the chemical ordering through controlling annealing conditions, such as temperature and duration. Our simulations show that distinct chemical ordering structures emerge in CrCoNi MEA when annealed at certain temperatures. These structures effectively repel interstitials and vacancies, resulting in a restricted diffusion region and, consequently, slower effective diffusion rates of entire system. Notably, diffusivity correlates directly with the degree of chemical ordering, which in turn is influenced by the annealing duration at a given temperature. This underscores the potential to interstitials and vacancies by modulating the degree of chemical ordering, achieved by fine-tuning the annealing temperature and duration.
We conclude by high-lighting the pivotal role of operating temperatures on diffusion, emphasizing that to preserve the slow diffusion effect, the operating temperature should remain well below the annealing temperature.



Computing system: SQUID General Purpose CPU nodes

node-hour	8,830 node-hour
memory used	250 GB
parallelize	4 nodes