Neural Network-Driven Atomistic Modeling of Chemical Ordering Kinetics and Their Impact on Diffusivity and Deformation in Multi-Principal Element Alloys

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The formation of local chemical order in multi-principal element alloys has been increasingly evidenced through recent experimental and theoretical studies. Given that chemical ordering can significantly alter the mechanical and functional properties of these alloys, tailoring chemical order presents a promising avenue for enhancing these properties. However, the specifics of the atomic structure and, crucially, its formation kinetics, remain poorly understood. This study employs a newly developed artificial neural network potential (ANNP)-driven atomistic simulation approach, including artificial-neural-network-accelerated kinetic-Monte-Carlo (ANN-kMC) simulations for vacancy diffusion, to precisely characterize both the chemical ordering structures and their formation kinetics in relation to annealing temperature and duration in CrCoNi alloys. Subsequently, we assess the impact of chemical ordering on nano-scale deformation and strength and interstitial/vacancy diffusion in CrCoNi alloys using ANNP-driven molecular dynamics and ANN-kMC simulations. Our findings elucidate a definitive connection between the degree of chemical ordering and the resultant strength and the point defect diffusion properties of the alloys.

Related publications:

- Yangen Li, Jun-Ping Du, Shuhei Shinzato, and Shigenobu Ogata, npj Computational Materials 10 (2024) 134.
- Le Li, Jun-Ping Du, Shigenobu Ogata, and Haruyuki Inui, Acta Materialia, 269 (2024) 119775.
- Jun-Ping Du, Peijun Yu, Shuhei Shinzato, Fan-Shun Meng, Yuji Sato, Yangen Li, Yiwen Fan, and Shigenobu Ogata, Acta Materialia, 240 (2022) 118314.
- Peijun Yu, Jun-Ping Du, Shuhei Shinzato, Fan-Shun Meng, and Shigenobu Ogata, Acta Materialia, 224 (2022) 117504.