Multi-Layer History-Dependent Generalized Stacking Fault Energy in High-Entropy Alloys

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Purpose To investigate the comprehensive deformation mechanism in chemically ordered high-entropy alloy (HEA) controlled by the theory of multi-layer history-dependent generalized stacking fault energies.

Outline
1. Construction of database for neural network interatomic potential (NNIP) using density functional theory (DFT) calculations.
2. Use molecular statics (MS) simulations to determine the various generalized stacking fault energies with history-dependence theory in chemically ordered high-entropy alloys.
3. Use kinetic Monte Carlo (kMC) method to simulate the microstructure evolution based on the nucleation theory and the history-dependent generalized stacking fault energy theory.

Result We found that the multiple-time slipping induces chemical short-range order (CSRO) collapse, leading to local shear softening owing to the history dependence of GSFE. By kMC simulations, we proposed a laminated microstructure evolution that involves twinning and hcp phase transformation which can be controlled by the chemical order of such alloy.

Computing system: Octopus

node-hour 1500 node-hour
parallelize 4 node

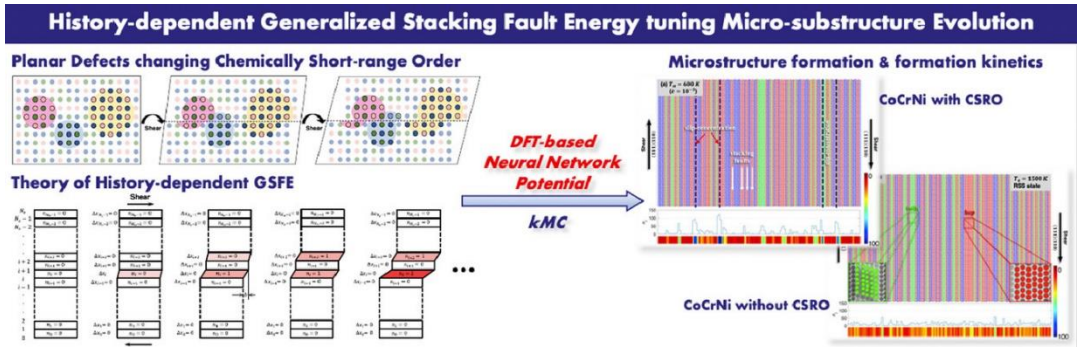

Fig 1. The history-dependent generalized stacking fault energies in the CoCrNi high-entropy alloys with chemical short-range order.