Kinetic Monte Carlo simulation of chemical short-range order formation kinetics in high-entropy alloys

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Purpose

The chemical short-range order (CSRO) affects the mechanical properties of high-entropy alloys (HEAs), so controlling the formation of CSRO enables tailoring of the mechanical properties of HEAs. However, the formation kinetics of CSRO is still unclear. In this study, we proposed a simulation framework to obtain the CSRO formation kinetics in HEAs.

Outline

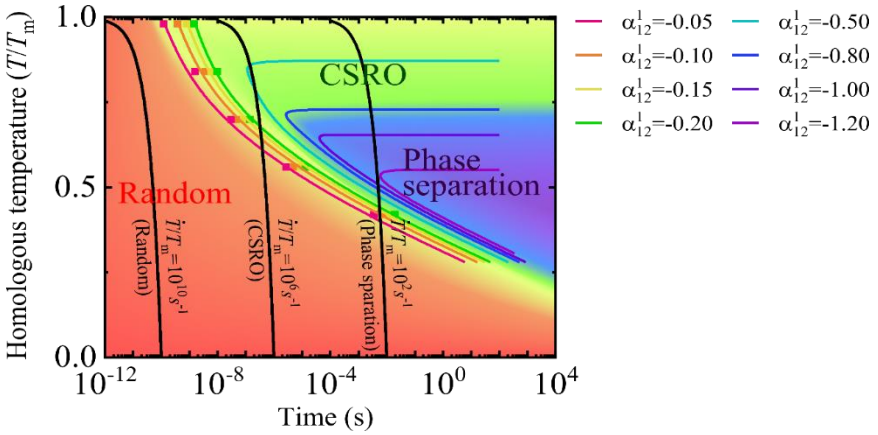
In this study, we designed a simulation framework to obtain the time–temperature–CSRO degree (TTC) diagram in HEAs using the kinetic Monte Carlo (kMC) method based on the assumption of the vacancy diffusion dominated CSRO formation process.

Result

A TTC diagram for a quinary HEA was obtained based on the Lennard–Jones model potential. The TTC curve shows the annealing time and temperature ranges/quenching rate range to form a certain degree of CSRO and avoid the occurrence of phase separation.

Computing system:

4000 node-hour
1GB/node memory used



TTC diagram for the quinary model HEA. Dots indicate data directly obtained by kMC and the colored lines are the fitting results of the data. Larger CSRO parameters (α_{12}^1) values imply phase separation. The solid black lines show temperature changes at constant quenching rates.