Accelerating Phase Diagram Prediction by Machine Learning Potentials

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Background: Phase-diagram prediction is very important for developing complex alloy systems, where experimental data are often limited. Machine-learning interatomic potentials (MLIPs) provide a practical way to accelerate this process by approximating first-principles accuracy at much lower computational cost. However, their limited transferability and statistical errors can reduce reliability in phase diagram predictions, especially for phase boundaries and transition temperatures.

Results: This research aims to improve the use of MLIPs for alloy phase-diagram prediction by benchmarking universal models, quantifying free-energy errors, and refining predictions through Bayesian statistics and optimal experimental design. This research shows that it is possible to reduce experimental effort while enabling faster and more reliable phase-diagram discovery using machine learning potentials, with a view toward future automated materials research workflows.

SQUID 汎用CPUノード群

ノード時間	4930 時間
使用メモリ	248 GB
並列化	1ノード 並列

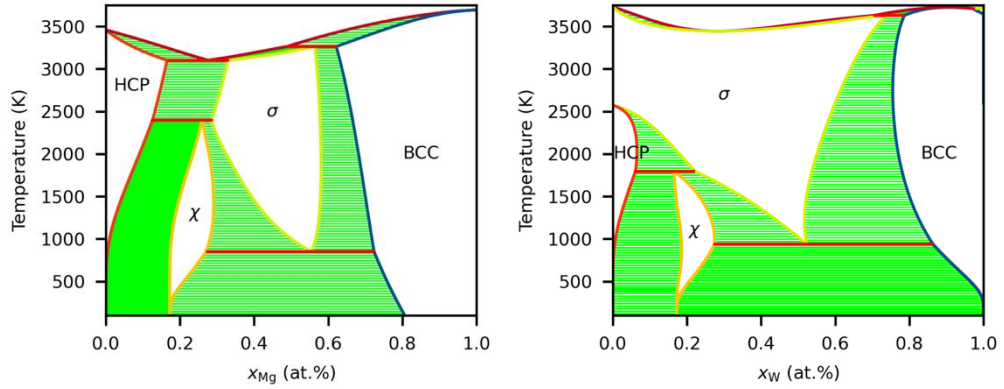

Figure Left: Phase diagram of W-Re from experimental assessment. Right: Phase diagram from MLIP (ESEN)