Using Kinetic Monte Carlo to Investigate NiAl Superalloys

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1 Overview

Nickel-based superalloys are used for their resistance to fatigue and creep, coupled with their strength. These properties require control at a microstructural level. However, formation of microstructures can cover timescales from femtoseconds up to thousands of hours. Continuum scale approaches cannot capture the movement of atoms through a system and classical molecular dynamics cannot access the time scales required to capture the formation of microstructures. This is where kinetic Monte Carlo (KMC) comes in as it can access longer time scales than molecular dynamics whilst also showing how the atoms move through the structure.

2 Method

KMC uses barrier heights to find change of state rates based upon transition state theory. These rates determine the timescale of time-evolution of the system and knowledge of them allows for longer timescales to be explored. Present research will use the LAMMPS[1] built-in nudged elastic band method to calculate energy barriers and a published potential[2] provided by the OpenKIM API[3]. The current project plan is modular, as seen in project design (4). This allows for the use of the potential in Monte Carlo simulations and KMC barrier height calculations. It also allows for development of a new potential which could be easily swapped in to model for a different alloy entirely.
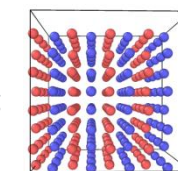
3 Current Work

Current work aims:
1. Verifying energy values against the published ones[2] to make sure the potential is working correctly.
2. Running a Monte Carlo simulation to make sure the real-world stable structures are recovered.
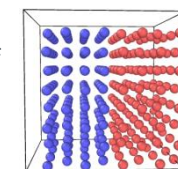
Why?
1. This is key due to the potential being used to calculate the barrier height in KMC and the rate of state transition in KMC is sensitive to barrier height.
2. This is making sure the structure coming out of the code is what happens in real life and there aren't effects like finite size stabilizing an unrealistic structure.

The current energy calculations are done on a fixed sized cell using LAMMPS[1] with the OpenKIM API for the potential. The calculations allow for relaxation of forces, positions and volume. LAMMPS[3] is accessed by a front-end python wrapper.
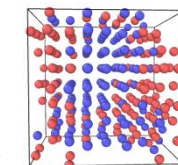
The python wrapper allow us to run a Monte Carlo simulation on a given structure and see what structure it stabilizes to. This is done by python randomly suggesting a swap and then it is accepted or rejected based on the energy calculated in LAMMPS using the OpenKim potential[2,3].
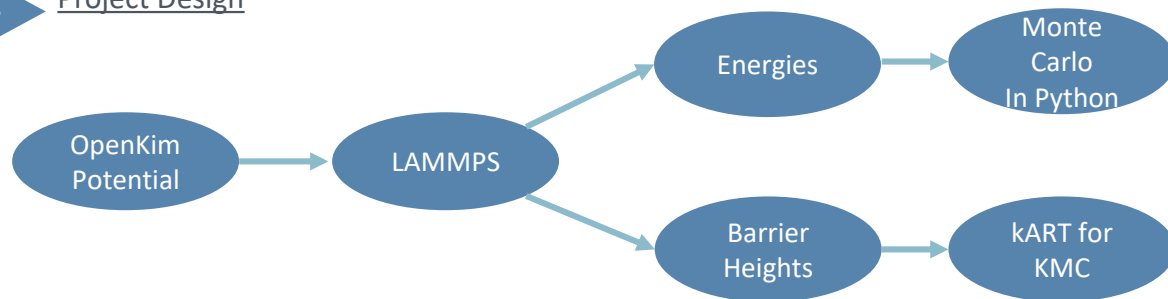

$L1_0$ Structure NiAl

Phase segregated NiAl

Random distribution of NiAl

4 Project Design

OpenKim Potential → LAMMPS → Energies → Monte Carlo In Python

LAMMPS → Barrier Heights → kART for KMC

5 Future Work

The next steps are:
- Use barrier height to calculate their rates.
- To use the kinetic Monte Carlo code kART[4] with the potential that is being used to propagate the system.

References:

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