Shape memory alloys

Shape memory alloys (SMAs) are a fascinating class of smart materials with applications ranging from stents to actuators. Among the known materials displaying this phenomenon, NiTi alloys have attracted the most attention due to their efficient shape recovery, mechanical robustness, and biocompatibility.

Phase transformation in NiTi

Structural phase transformation between high temperature and low temperature phases in NiTi are responsible for these interesting shape memory and super-elasticity properties.

Simulation details

Calculations were performed using molecular dynamics (MD) simulation implemented in the LAMMPS software package.

The interatomic interactions were captured through the Finnis Sinclair type EAM (embedded atom method) developed by Lai and Liu.

The temperature and pressure were controlled using Nose-Hoover thermostat algorithm and Parrinello-Rahman methods.

Effect of Point Defects on the Phase Transformation of NiTi Shape Memory Alloy

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Conclusions

1. MD simulation is a viable method to study the effect of point defect on phase transformation in NiTi.
2. Both vacancy and anti-site defect resulted in lower transformation temperature and angle.
3. This suppression is mostly through a pinning mechanism.

References


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