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

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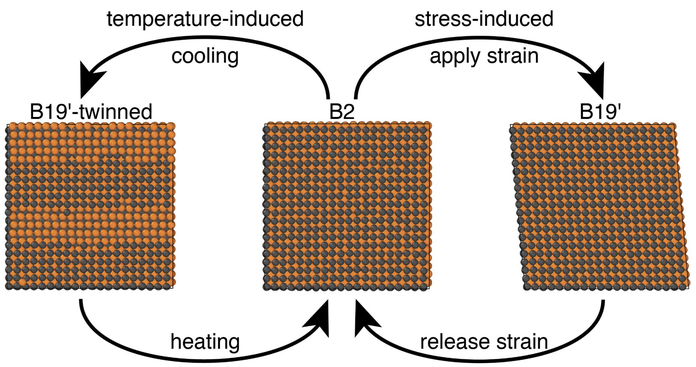
Shape memory alloys

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.



High temperature phase B2 (austenite) has a cubic *CsCl-type* crystal structure while the low temperature phase B19’ (martensite) is monoclinic.

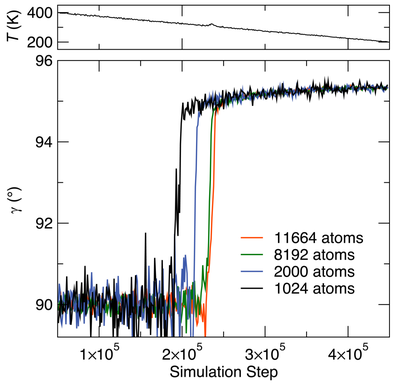
Simulation details

Calculations were performed using molecular dynamics (MD) simulation implemented in the LAMMPS software package[1]

The interatomic interactions were captured through the Finnis Sinclair type EAM (embedded atom method) developed by Lai and Liu[2].

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

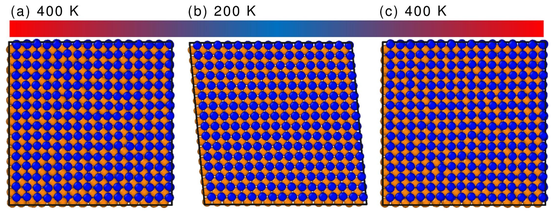
Effect of simulation size on phase transformation

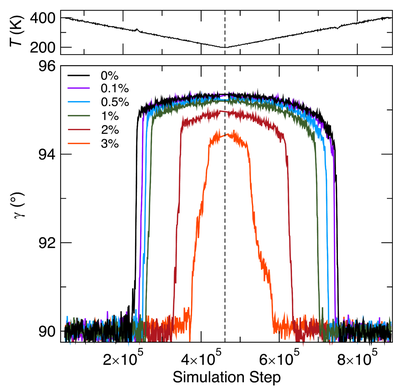


The abrupt change in angle indicates the transformation to monoclinic structure.

The transformation temperature does not change much after 8192 atoms simulation size which was picked for the further calculations due to the compromise between accuracy and computation cost.

Introducing vacancies



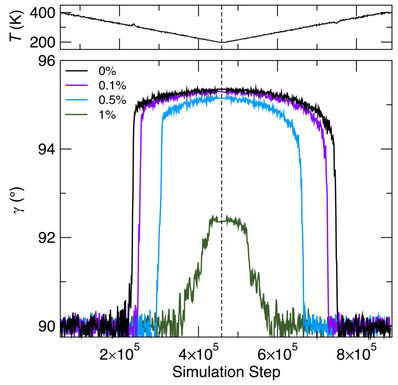


Increasing the concentration of vacancies leads to a substantial decrease in the phase transformation temperature

Suppression of γ is also evident

This is duo to the vacancies inhibiting the transformation by reducing the shear component.

Introducing anti-site defects



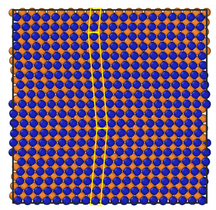
Increasing the concentration of anti-site leads to a more substantial decrease in the phase transformation temperature

Significant suppression of γ is also evident

Local change in the concentration of Ni or Ti produces elemental islands (FCC or HCP) in the matrix which prefer to remain in the B2 crystal structure energetically

Twinning

Further increasing the simulation size, 16000 atoms, resulted in a twinned structure. The twinning is expected and is in agreement with experiment



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

1- S. Plimpton , J. Comput. Phys. 117, 1 (1995).
2- W. S. Lai and B. X. Liu , J. Phys.: Condens. Matter 12, L53 (2000).
3- W. G. Hoover , Phys. Rev. A 31, 1695 (1985).

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