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A molecular dynamics study on the effect of precipitate on the phase transformation in NiTi

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Research Question

Considering different crystallographic orientations, how phase transformation of single-crystal NiTi alloy can be affected by the presence of precipitate?

Introduction

NiTi being one of the most important shape memory alloys has found increasing applications in industries like aerospace and biomedical. This popularity arises from its shape memory effect that is the capability of recovering the pre-deformed shape when heated, and superelasticity which is the reversible elastic behavior caused by solid-state phase transformation (see Fig. 1). It has been shown that the presence of inclusions can affect thermo-mechanical response in NiTi. To perform an optimum material design and taking advantage of desired properties of NiTi for different applications, these aspects of NiTi's behavior should be understood well. In this study, the effect of a common type of inclusion (precipitate) on the stress-induced and temperature-induced phase transformations in NiTi is studied using molecular dynamics (MD) simulations.

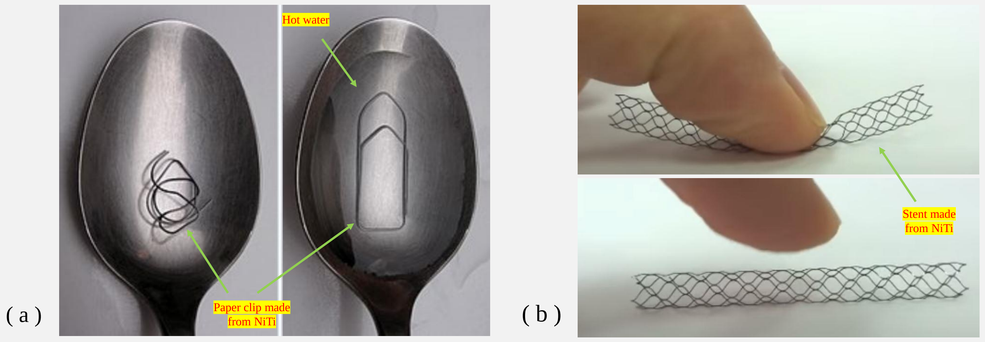

Fig. 1 – a) Shape memory effect in NiTi: Deformed paper clip recovers its original shape in the hot water. b) Superelasticity in NiTi: Reversible elastic behavior helps inserted collapsed stent in the artery to expand to its original shape.

Methods

Open-source molecular dynamics code (LAMMPS) [1] was employed for simulations. In order to represent the energy differences between austenite (B2) and martensite (B19′) phases during a phase transformation, MEAM potential developed by Ko et al. [2] was used which is one of the critical necessities of the MD simulation. In order to model Ni_4Ti_3 precipitate in the NiTi matrix, first an Ni_4Ti_3 ellipsoid, having a rhombohedral crystal structure, was modeled as the precipitate and then it was embedded into the center of the austenitic NiTi cube. The minor axis of the precipitate was along [111] crystal orientation (Fig. 2). To obtain phase transformation temperatures for the pure NiTi and precipitated models, a cycle of cooling (from a high temperature at which the material was austenite) and heating process was applied to the models. Initially, B2 austenitic NiTi model was equilibrated at 500 K and then the temperature was reduced gradually to 100 K. Afterwards, the temperature was increased gradually to 500 K. In order to see the effect of the precipitate on the mechanical behavior of NiTi matrix, a compressive load was applied in a stress-controlled condition to the models with and without precipitate. The load was gradually applied from 0 to 2 GPa and then gradually unloaded to 0 GPa. The same load was applied in other directions ([201], [101], [102] and [001]) to study the effect of precipitate in different crystallographic directions.

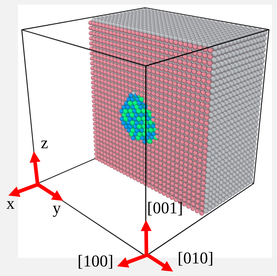

Fig. 2 – The NiTi model with precipitate (the model is cut in half for better visualization)

Results

Observing the change in atomic volume during cooling and heating is a useful method to determine the phase transformation temperatures of NiTi from MD simulations. As can be seen in Fig. 3, the presence of the precipitate did not impose a noticeable change on the transformation temperatures (except M_f) of both NiTi models. Although, there were some small differences in twinning planes of the two models, those differences did not affect the volume of the model significantly. In Fig. 4, the stress-strain curve of the models subjected to compressive stress as well as their microstructure are shown (pink atoms belong to martensite and blue ones represent austenite). It was observed that slower rate of reverse phase transformation occurs due to the presence of precipitate, which hinders the reverse phase transformation, and thus causes a larger hysteresis loop in the precipitated NiTi. In addition, the precipitated model exhibits a higher loading transformation stress level of ~50 MPa. It was also seen that the effect of precipitate on the stress-strain response is more pronounced in ⟨100⟩ family of crystallographic directions. It can be interpreted that the local stress field that occurs in the vicinity of precipitate due to the lattice mismatch between the precipitate and the matrix is larger in these directions.

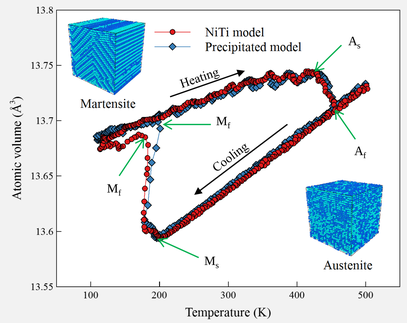

Fig. 3 - Atomic volume at different temperatures in a cooling-heating cycle. Green arrows indicate the instance of start and finish of phase transformations.

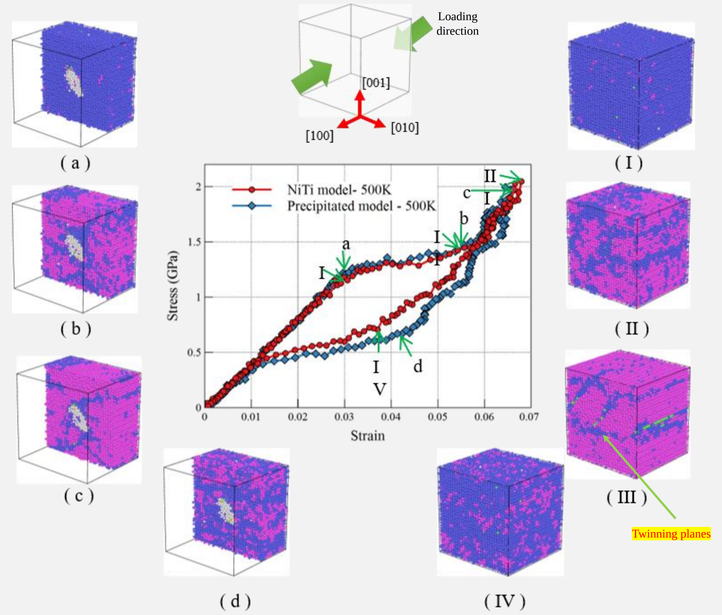

Fig. 4- Stress-strain curves of NiTi and precipitated model at 500 K and corresponding atomic structures at different strain levels

Conclusions

The following conclusions can be drawn from this study:

1) The presence of rhombohedral Ni_4Ti_3 precipitate does not have a noticeable effect on the thermally-induced phase transformation and, thus, transformation temperatures of NiTi.

2) At 500 K where the material is fully austenitic, the rhombohedral Ni_4Ti_3 precipitate causes a larger hysteresis loop for NiTi subjected to compression in [100] direction and subsequently more energy dissipation capability.

3) For superelastic NiTi (at 500 K) and among different loading directions studied in this work, the effect of the precipitate was more pronounced in ⟨100⟩ family of crystallographic directions.

References

1. Plimpton, S., Fast Parallel Algorithms for Short-Range Molecular Dynamics. Journal of Computational Physics, 1995. 117(1): p. 1-19.
2. Ko, W.-S., B. Grabowski, and J. Neugebauer, Development and application of a Ni-Ti interatomic potential with high predictive accuracy of the martensitic phase transition. Physical Review B, 2015. 92(13): p. 134107.