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Influence of compound twinning on Young's moduli in NiTi martensite

Petr Šesták[a], Miroslav Černý, and Jaroslav Pokluda

Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, 616 69 Brno, Czech Republic

Abstract. NiTi shape memory alloy has been widely used in many engineering applications (e.g. mechatronic devices, medical tools, seismic sensors etc.). In this work, the Young's moduli of twinned NiTi martensite in selected crystallographic directions are calculated from first principles and compared with previous data for perfect (untwinned) NiTi structure. The obtained results show that the selected twinning mode does not have a significant influence on the Young's moduli and, thus, their reduction observed in some experiments is probably caused by changes in martensitic microstructure (arrangement of twinning variants).

1 Introduction

The shape memory effect has been first observed in 1951 on Au-Cd alloy [1]. The next shape memory alloy (SMA), In-Tl [2], has been discovered a few years later. However, the significant research of SMAs has started in 1963 when NiTi SMA was discovered [3]. The NiTi SMA is used in various applications, e.g. mechatronic actuators [4], medicine (stents, bone implants) [5] or seismic devices [6] due to their very good shape memory characteristics. The shape memory effect is caused by transformation from the martensitic (monoclinic B19') to the austenitic (cubic B2) phase (see Fig. 1) and vice versa and can be started by an external deformation or a temperature change. This particularly means that, after a deformation-induced shape change in the martensitic condition, the SMA returns to its original geometrical shape when being warmed up to the austenitic state. Such a behavior is facilitated by a reversible creation and vanishing of selected twinning variants in the domain-like martensitic microstructure. There are several possible types of phase transformations depending on a particular alloy composition. An extensive overview of a current state of the art can be found in the paper by Otsuka and Ren [7]. There are also several papers investigating this alloy using the first principles (ab-initio) calculations [8–12] focused on its structural, electronic or elastic characteristics.

In the case of SMAs, the transition from elastic to pseudoplastic behavior is of a great practical importance. The elastic response of materials to uniaxial strains close to equilibrium state can be characterized by the Young's moduli. However, the experimental data are measured within a wide range depending on the applied deformation. For very small values of strain ($\varepsilon \approx 10^{-6}$) is the corresponding range of obtained Young's moduli $E \approx 90 \div 130\,\mathrm{GPa}$, whereas by application of higher strain values ($\varepsilon \approx 10^{-4}$) $E \approx 60 \div 70\,\mathrm{GPa}$ was determined [13]. The measured values of E in lower strain experiments are in agreement with our previously published theoretical (ab-initio) data [12] of perfect NiTi martensite which are also very close to the range of $90 \div 130\,\mathrm{GPa}$.

[a] e-mail: sestak@fme.vutbr.cz

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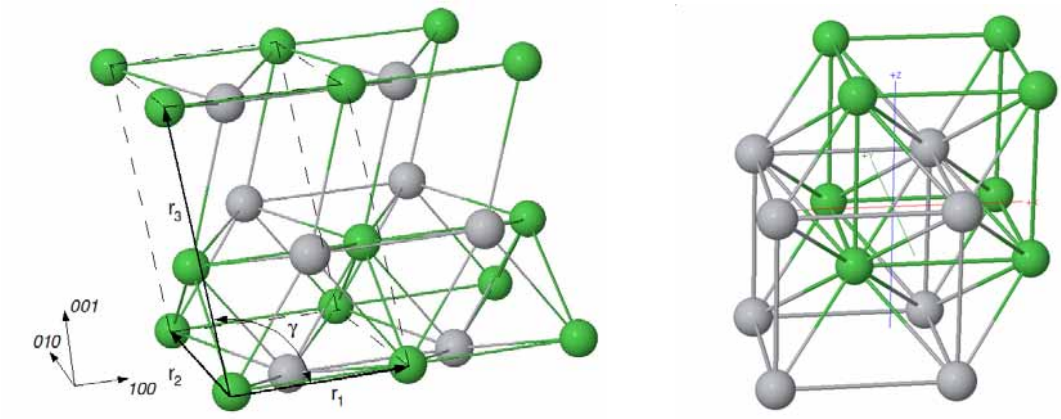

Fig. 1. Martensitic (monoclinic structure B19') and austenitic (cubic structure B2) phase of NiTi shape memory alloy.

The main aim of this work is to calculate Young's moduli of a twinned martensite structure and to assess an influence of the twins on elastic response of martensite by comparing the obtained values with results for an ideal untwinned structure.

2 Computational details

2.1 Computational program code

The total energy U_{tot} of the studied system and the stress tensor $\hat{\sigma}$ were computed by the Abinit program code [14–16]. Abinit is an efficient tool for electronic structure calculations based on density functional theory [17] and pseudopotential approach. The program has been developed by the team of Prof. Xavier Gonze at the Université Catholique de Louvain, and is distributed under GNU General Public License. Another additional package including pseudopotentials together with its generators, manuals, tutorials, examples, etc. are available in [18].

The calculations were performed using GGA PAW pseudopotentials [19] and the cutoff energy was set to 270 eV. The solution was considered to be self-consistent when the energy difference of three consequent iterations became smaller than 1.0 μeV.

2.2 Evaluation of Young's moduli

The elastic response to uniaxial loading expressed by Young's modulus can be computed either from the dependence of the total energy U_{tot} (per unit cell) on the applied strain ε (along the particular crystallographic direction) or from the stress – strain response $\sigma(\varepsilon)$. In the former case, the Young's modulus E can be calculated using the relation

$$E = \frac{1}{V_0} \frac{d^2 U_{tot}}{d\varepsilon^2}, \tag{1}$$

where V_0 is the unit cell equilibrium volume. The latter case uses the related components σ of the computed stress tensor (after all the other components were relaxed to negligible values) as

$$E = \frac{d\sigma}{d\varepsilon}. \tag{2}$$

In the present work, both approaches were used to compute the Young's moduli and their results agreed mostly within 1–4%.

2.3 Construction of the super-cell

Several types of twinning modes can be found in the NiTi martensite. The twins are described by elements of twinning and according to these elements they can be separated into three different groups (Type-I, Type-II and compound). A detailed specification of NiTi martensite twinning modes can be found in Ref [7]. In this particular study, the compound twinning mode (100) has been selected for computation of the Young's moduli due to the fact that the simulation basis is simpler than that for the other twinning modes.

The simulation cell was build as a super-cell composed of eight primitive cells (of two different bases). The first base corresponds to a standard B19' martensite and the other one represents a tilted base of B19' martensite. The tilted base was created by giving the translation vector r_3 (Fig. 1) a tilt that leads to a decrease of the γ angle – see the scheme in Fig. 2.

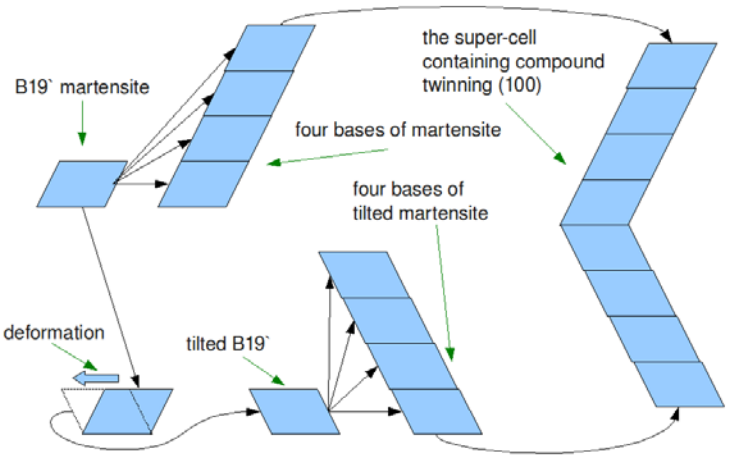

Fig. 2. The process of building the computational super-cell containing a compound twin (100).

The resulting simulation cell is displayed in Fig. 3 on the left. However, this cell was not still used for computations of Young's moduli E because the values of the stress tensor and forces acting on individual atoms at the twin interface were too high. For this reason, the translation vectors describing the cell as well as the ionic positions at the twin interface have been optimized using a relaxation procedure that guarantees the stress values lower than 500 MPa and the atomic forces below 10^{-1} eV/Å. It is very difficult to relax the stresses and forces to lower values because the cell contains an interface between two different variants of B19' martensite and the optimization process must be partially constrained to preserve the twinned structure (without any restriction, the optimization procedure tends to lead the structure to an untwinned martensite).

The optimized simulation cell is displayed on the right hand side of Fig. 3. As can be seen, the optimized atomic positions in the vicinity of the interface are arranged along the {100} plane, making the interface almost flat in agreement with data available in Ref. [11]. The optimized cell was finally used for a computation of the Young's moduli of the twinned structure.

3 Results and discussion

The computed theoretical Young's moduli E of the twinned NiTi martensite for [100], [010], [001], [101], and [10$\bar{1}$] directions are listed in Tab. 1 along with the previously computed theoretical data [12] for a perfect crystal. As can be seen, the theoretical data for both the twinned and the perfect martensite lie within the range of $90 \div 130$ GPa. This correspondence indicates that the selected twinning mode does not exhibit any significant influence on the Young's moduli E.

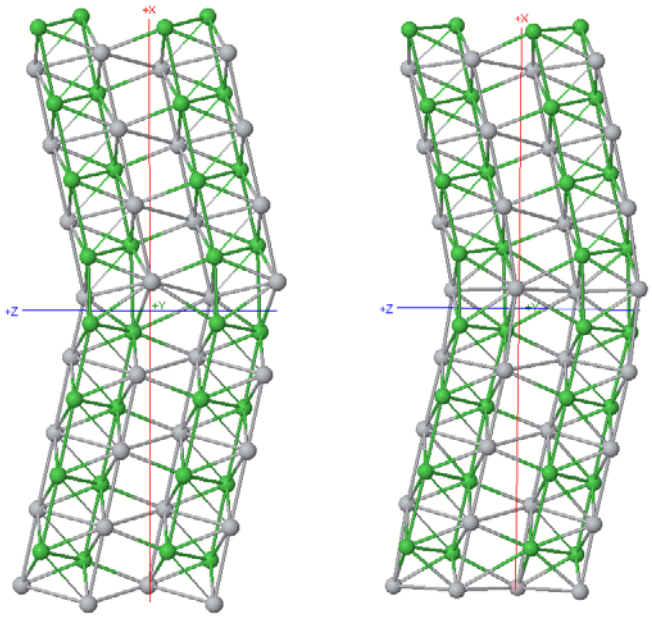

Fig. 3. The super-cell containing compound twin (100) before optimization of ionic positions at the interface (on the left) and after the optimization (on the right).

Table 1. Theoretical values of Young's moduli E for twinned NiTi martensite along with previously computed theoretical data [12] for perfect NiTi martensite crystal. The available experimental data [13] are also included.

Young's moduli	E_{100} [GPa]	E_{010} [GPa]	E_{001} [GPa]	E_{101} [GPa]	$E_{10\bar{1}}$ [GPa]
B19' twinned	98	113	116	123	126
B19' perfect crystal	96	124	126	-	-
B19' exp. ($\varepsilon \approx 10^{-6}$)			$90 \div 130$		
B19' exp. ($\varepsilon \approx 10^{-4}$)			$60 \div 70$		

All the presented theoretical values of the Young's moduli E are in a good agreement with experimental data. Of course, the relevant experimental data of the Young modulus E for the B19' structure belong to the range of $90 \div 130$ GPa which has been measured when applying the deformation $\varepsilon \approx 10^{-6}$. Such small values of ε can guarantee no change of twin structure in NiTi martensite while the higher values of ε may cause changes in the twin configuration and lead to lowering the Young's moduli E.

4 Conclusion

First principles calculations of an elastic response to uniaxial loadings in five particular crystallographic directions were performed for a model of twinned NiTi martensite. The model of twinned structure was based on a partially optimized super-cell composed of eight primitive B19' cells optimally strained and arranged to represent an example of compound twinning mode. The calculated theoretical values of the Young's moduli are compared with previously published data for a perfect martensite crystal. It was found that the selected compound twinning mode does not have a significant influence on the computed values. Since the present theoretical data are in a good agreement with available experimental results for low strain

measurements, the reduction of Young's moduli observed in some experiments seems to be a result of an rearrangement of twinning variants.

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