Ideal strength of twinned and perfect NiTi martensite crystal

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Abstract This paper is focused on the determination of the ideal (theoretical) tensile strength of the NiTi martensite crystal with B19' and BCO structures which contain (100) compound twins. For comparison, the strength of a perfect austenitic B2 structure is also studied. The model of the twinned martensite is represented by a supercell containing 40 atoms (20Ni:20Ti) arranged in two variants of the martensite. The results show that the presence of twins slightly decreases the ideal strength of NiTi martensite. The ideal strength of the B2 structure is three-times higher than that of the BCO one.

Keywords NiTi SMA, twinning, theoretical strength, ab initio

1. Introduction

The shape memory alloys (SMA) represent advanced materials usable in many industrial as well as medical applications owing to their shape memory effect which is based on transformations between austenitic and martensitic phases. The most frequently used SMA is a binary alloy with a nearly equiatomic proportion of nickel and titanium (NiTi). The NiTi alloy crystallizes either into a high temperature B2 (austenite) or a low temperature B19' (martensite) structure. An extensive overview regarding the NiTi SMA can be found in the paper of Otsuka [1].
There is, however a disagreement between experiment and theory since ab initio simulations predict, as a structure with the lowest total energy E_{tot} the base centered orthorhombic structure (BCO) instead of the experimentally observed monoclinic B19' one [2]. This disagreement raises a question why the theoretical simulations do not predict and confirm the experimentally observed martensitic structure. One of possible explanations is that the experimental results were measured on a polycrystal while the theoretical models consider a perfect crystal that does not contain the planar crystallographic defects, like twins or dislocations. Indeed, the real NiTi martensite always contains twins and, therefore, it is necessary to include these defects into the theoretical model. In our previous ab initio study we considered a sample of the (100) compound twins in NiTi martensite. Received results revealed that presence of the selected twins can significantly contribute to stabilization of the B19’ structure against the BCO one. Hence, the knowledge of the twinning in NiTi SMA at atomistic level is important for deeper understanding the ongoing processes (detwinning, martensitic transformation, etc.) in this unique material.
In this theoretical study we present the ab initio simulations of the (100) twinned NiTi martensite subjected to a uniaxial tensile loading that is oriented perpendicular to the twinning planes.

2. Theoretical model of the twinned NiTi martensite

2.1. NiTi twinned martensite

The studied theoretical model of the (100) compound twins in the NiTi martensite is represented by a supercell containing 40 atoms (20Ni:20Ti) arranged in two variants of the martensite. From now on, this basis will be referred to as TSC – twinned supercell. This TSC is identical to that already published in our previous research paper [3] that also contains a detailed description the TSC construction. The sample of the (100) twinned structure is depicted in Fig. 1.

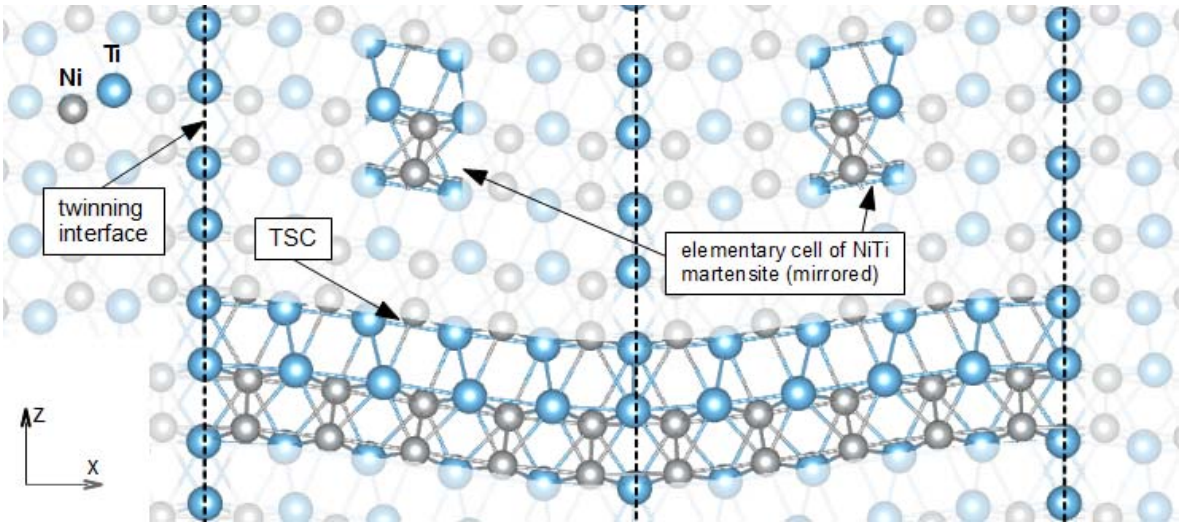

Figure 1. The sample of (100) twinned NiTi martensite with marked twinned supercell (TSC), both martensite variants and twinning interfaces. The tensile loading was applied parallel to the z axis.

2.2. Theoretical simulations

The ab initio simulations were performed within the density functional theory (DFT) developed by Kohm and Sham [4]. We used the VASP code (Vienna Ab initio Simulation Package) [5, 6] as a particular implementation of DFT to determine the total energy (E_{tot}) of the studied system, the stress tensor (σ_i in Voigt notation) and the forces (F) acting on individual atoms. The VASP uses the pseudopotential approach that represents a very efficient way how to reliably describe the valence electrons.

In the present study we utilized the PAW (Projector Augmented Waves) [7] pseudopotential treating p-electrons of Ti as valence and the exchange correlation energy by mean of the GGA (Generalized Gradient Approximation) with parametrization of Perdew Wang [8]. The cut-off energy restricting the number of plane waves in the basis set was 500 eV and the solution is considered to be self consistent when the difference of two subsequent total energies is lower than 1.0×10^{-8} eV. Meshes containing 1×13×13 (for TSC), 19×13×13 (for BCO) and 19×19×19 (for B2) of equidistantly spaced k-points were constructed for integration over the Brillouin zone.

The modeled deformation of a crystal lattice is represented by a uniaxial distortion of TSC in the selected direction that is perpendicular to the twinning interfaces. The relaxation procedure was applied during the entire deformation process to achieve the Poisson contraction (relaxation of the lateral stress tensor components). This relaxation means alternating the optimization of the translation vectors with optimization of the atomic positions until the relaxed stress tensor components reached values below 200 MPa and forces between individual atoms were lowered to 1×10^{-2} eV/ Å.

3. Results

3.1. Structure optimization

The uniaxial deformation begins from the equilibrium state and therefore it was necessary to determine lattice parameters for all studied structures. The lattice parameters of TSC were taken from our previous ab initio study [3] whereas the lattice parameters of the BCO and the B2

structures were obtained by a full optimization of those experimentally measured. These parameters are listed in Table 1 along with the experimental data [1, 9]. Comparing the presented ab initio data with those published in literature one can note a good agreement. This proves that the selected VASP settings are sufficient for reliable ab initio simulations.

Table 1. The computed equilibrium lattice parameters of the NiTi SMA. The table also contains the experimental and the theoretical data that are available in literature.

Structure	a_0 / Å	b_0 / Å	c_0 / Å	β / [°]
TSC [3]	28.7	4.11	4.65	90.0
BCO present *	2.94	4.00	4.93	107.3
BCO [2]	2.85	3.92	4.82	107.2
B19' experiment [9]	2.90	4.11	4.65	97.8
B2 present	3.00	3.00	3.00	90.0
B2 experiment [1]	3.02	3.02	3.02	90.0

3.2. Theoretical tensile strength

The investigated structures were subjected to a uniaxial loading in the ⟨100⟩ direction. The deformation path started with the equilibrium lattice parameters and continued until the tensile stress exceeded its maximal value. The tensile stress σ_1 is plotted in Fig. 2 as a function of the strain ε_1 for all studied structures. The theoretical strengths of the TSC and the perfect martensite are identified with the maxima in the stress-strain dependences (see Fig. 2a) since behind these maxima, the structures transform into different ones. Fig. 2b contains the stress-strain dependence for the austenite where two maxima can be found. Since, there is no structure change during the deformation we consider the global maximum as the ideal strength of the austenite.

The highest theoretical strength σ_1 = 34.5 GPa corresponds to the B2 austenite whereas the lowest value of 7.6 GPa to the TSC structure. The value of 8.8 GPa for the BCO structure is rather close to that computed for the TSC but, indeed, the presence of selected twins slightly reduce the strength of the NiTi martensite. The results also revealed that the computed theoretical strengths for both the

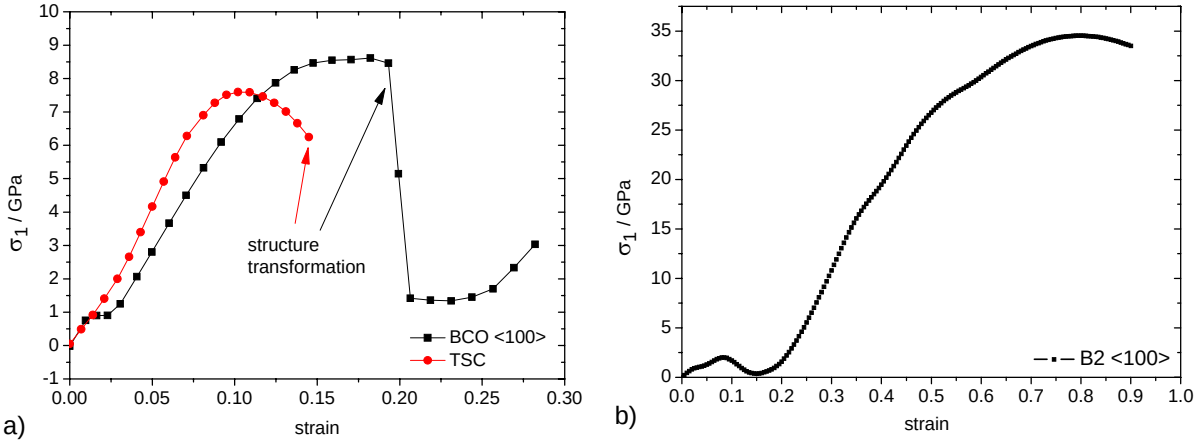

Figure 2. The dependence of the tensile stress σ_1 on the axial strain ε_1 for the twinned structure (TSC) and the perfect structures (B2 and BCO) of NiTi. The direction of deformation is perpendicular to the twinning interfaces.

TSC and the BCO lattice are significantly different from that for the austenite which is three times higher. A similar difference can be found when comparing the critical strain values. All the computed theoretical data are summarized in Table 2.

Table 2. The theoretical tensile strengths σ_{max} of the studied structures along with strain values.

Structure	σ_{max} / GPa	ε
TSC	7.6	0.106
BCO	8.8	0.219
B2	34.5	0.795

4. Conclusion

The theoretical tensile strength of the twinned NiTi martensite in the ⟨100⟩ direction was computed using the ab initio simulations and compared with those of perfect martensite and austenite structures. The results revealed that the presence of twins in the NiTi martensite only slightly reduces its theoretical strength. The results also show that the strength of the austenitic crystal is three times higher than that of the martensitic one.

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