UDC 539. 4

Elastic Properties of B19' Structure of NiTi Alloy under Uniaxial and Hydrostatic Loading from First Principles

P. Šesták,[1,a] M. Černý,[1,b] and J. Pokluda[1,c]

[1] Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

[a] sestak@kn.vutbr.cz, [b] cerny.m@fme.vutbr.cz, [c] pokluda@fme.vutbr.cz

The uniaxial and hydrostatic deformations of martensitic structure B19' of NiTi shape memory alloy are studied using first-principles calculations. The bulk and Young's moduli and the theoretical strength under uniaxial tension and hydrostatic loading are computed from crystal response to applied deformations. The behavior of angle β of the B19' structure was investigated along the whole deformation path. The computed values of Young's moduli are compared with available experimental results. The results obtained complement and extend the already known characteristics of NiTi alloy.

Keywords: NiTi, B19', shape memory alloy, first principles, ab-initio, elastic properties, theoretical strength, uniaxial and hydrostatic deformation.

Introduction. The shape memory alloys (SMA) are important materials for many industrial as well as medical applications owing to their shape memory effect. This effect is connected with a transformation between martensitic and austenitic structure, which can be started by an external pressure or temperature. There are several types of the transformations, depending on a particular alloy.

The nickel-titanium alloy is one of the most important types of SMA. It is widely used in medicine (stents, bone implants, etc.). The NiTi alloy can transform from the monoclinic B19' (martensitic) to cubic B2 (austenitic) structure and vice versa. An extensive overview of a current state of the art can be found in the paper by Otsuka and Ren [1].

The aim of this work is to compute the Young E and bulk B moduli and the theoretical strengths under uniaxial and hydrostatic (isotropic) loading. The Young modulus has been computed for three crystallographic directions (E [100], E [010], and E [001]) parallel to primitive translation vectors ($\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$) shown in Fig. 1. The dependence of the β angle (between $\mathbf{r}_1$ and $\mathbf{r}_3$ vectors) on the applied uniaxial deformation has been also investigated.

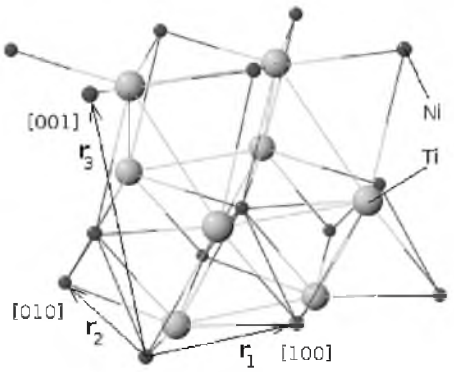

Fig. 1. The martensitic structure (B19') of NiTi alloy with marked crystallographic directions.

Electronic Structure Computations. All quantities of interest are computed from the total energy E_{total} of the system at hand as a function of an appropriate deformation and from the Hellman–Feynman stress tensor.

The total energies and stresses were computed by the Abinit program code. Abinit is a great tool for electronic structure calculations developed by the team of Prof. Xavier Gonze at the Universitй Catholique de Louvain [2, 3], which is distributed under the GNU General Public License. Another additional package including pseudo-potentials [4] together with its generators, manuals, tutorials, examples, etc. is available at [5].

The calculations were performed using GGA norm-conserving pseudo-potentials and the cutoff energy was set to 1000 eV for computations of elastic moduli and 800 eV for theoretical strength evaluation. The solution was considered to be self-consistent when the energy difference of three consequent iterations became smaller than 0.1 μeV for computation of elastic properties and 1.0 μeV for the theoretical strength.

During the uniaxial deformation the structure must be relaxed in order to allow the Poisson contraction. The relaxations were made by an external procedure utilizing the Hellman-Feynman stress tensor [6] computed by the Abinit code.

Computation of Elastic Moduli and Theoretical Strength. The Young's modulus can be computed as

$$E = \frac{1}{V_0}\frac{d^2 E_{total}}{d\varepsilon^2}, \tag{1}$$

where ε is the relative uniaxial deformation, $\varepsilon = a/a_0 - 1$. Similarly, the uniaxial stress can be evaluated as

$$\sigma^{uni} = \frac{1}{V_0}\frac{dE_{total}}{d\varepsilon}. \tag{2}$$

The bulk modulus and the hydrostatic stress were calculated according to the relations

$$B = \frac{1}{V_0}\frac{d^2 E_{total}}{dv^2} \tag{3}$$

and

$$\sigma^{hyd} = \frac{1}{V_0}\frac{dE_{total}}{dv}, \tag{4}$$

where v is the relative volume $v = V_0/V - 1$. Both stresses approach their maxima at the points of inflection of $E_{total}(\varepsilon)$ or $E_{total}(v)$ dependences. If no other instability appears before reaching the points, their maximum values specify the corresponding theoretical strength values σ_{id}.

Results. The experimental and ab-initio values of primitive translation vectors and β angle of the B19' structure are displayed in Table 1. The ab-initio results predict slightly larger values than those found in experiment. This overestimating of translation vectors is a typical effect of GGA pseudopotential type but the related errors are smaller than 5%.

Table 2 contains the computed values of the Young's and bulk moduli of the martensitic B19' and austenitic B2 structures. As can be seen, the Young's moduli of B19' are higher than those of the austenitic B2 structure for all the directions studied. These results are in contrast with experimental and finite element method (FEM) values, which predict the Young's modulus of martensite to about one-third to one-half of that of austenite [7].

This can be explained by the fact that the experimental data were measured on polycrystalline samples at finite temperatures, whereas the atomistic model does not allow

for any shear deformation of martensite variants, and describes a homogeneous deformation of a single crystal at the absolute zero temperature. On the other hand, the bulk modulus for the B19' structure is lower than that for the B2 structure. Table 3 contains values of the theoretical strength for all applied deformations.

T a b l e 1

The Experimental [1] and Ab-Initio Crystallographic Data for B19' Structure

Parameter	Experimental	Ab initio
a_0, Å	2.889	3.007
b_0, Å	4.120	4.121
c_0, Å	4.622	4.813
β, deg	96.8	100.6
V, Å^3	54.63	58.61

T a b l e 2

The Elastic Moduli of the B19' and B2 Structures, as Obtained from Present Ab-Initio Calculations along with Experimental [7] Results

Structure\moduli	E [100], GPa	E [010], GPa	E [001], GPa	B, GPa
B19' (ab-initio)	96	124	126	137
B2 (ab-initio)	72	72	72	155
B2 (FEM)	69	69	69	–

T a b l e 3

Computed Values of the Theoretical Strength of the B19' and B2 Structures

Structure\theoretical strength	σ_{id}^{uni} [100], GPa	σ_{id}^{uni} [010], GPa	σ_{id}^{uni} [001], GPa	σ_{id}^{hyd}, GPa
B19' (ab-initio)	19.0	27.5	20.7	22.1
B2 (ab-initio)	–	–	–	24.0

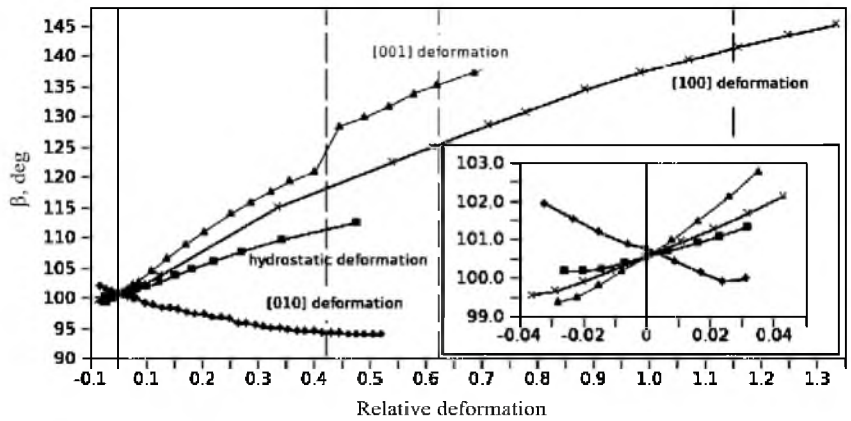

Fig. 2. The angle β as a function of applied deformation. The detail of the range close to the nondeformed state is depicted at the bottom right.

Under an applied deformation, the angle β changes as a result of the relaxation procedure. The dependence of the β angle on the applied deformation is shown in Fig. 2.

The points related to the theoretical strength are also marked (the inflection point in the dependence $E_{total}(\varepsilon)$ resp. $E_{total}(v)$ by dashed vertical lines. One can see that the angle β grows for all the deformation paths except for the [010] direction. Note that the [010] direction is perpendicular to vectors $\mathbf{r}_1$ and $\mathbf{r}_3$; therefore, the decrease in the β angle during the [010] deformation is to be expected.

Conclusions. The uniaxial and hydrostatic deformation of martensitic structure B19' of NiTi shape memory alloy was studied using first-principles calculations. The results of computations of Young's and bulk moduli are as follows: E [100] = 96 GPa, E [010] = 124 GPa, E [001] = 126 GPa, and B = 137 GPa. During the uniaxial and hydrostatic deformation the theoretical strengths were computed for all cases of applied deformations: σ_{id}^{uni} [100] = 19.0 GPa, σ_{id}^{uni} [010] = 27.5 GPa, σ_{id}^{uni} [001] = 20.7 GPa, and σ_{id}^{hyd} = 22.1 GPa. The Young moduli of B19' are higher than those of the austenitic B2 structure for all the directions studied and the bulk modulus for the B19' structure is lower than that for the B2 structure. The angle β grows for all deformation paths except for the [010] direction.

Acknowledgments. This research was supported by research projects GA 106/05/H008 and MSM 0021630518.

1. K. Otsuka and X. Ren, *Prog. Mater. Sci.*, **50**, 511 (2005).
2. X. Gonze, J.-M. Beuken, R. Caracas, et al., Comp. Mater. Sci., 25, 478 (2002).
3. X. Gonze, G.-M. Rignanese, M. Verstraete, et al., *Zeit. Kristallogr.*, **220**, 558 (2005).
4. M. Fuchs and M. Scheffler, *Comp. Phys. Communicat.*, **119**, 67 (1999).
5. http://www.abinit.org
6. D. R. Hamann, X. Wu, K. M. Rabe, and D. Vanderbilt, *Phys. Rev. B*, **71** (2005).
7. X. M. Wang and Z. F. Yue, *Comp. Mater. Sci.*, **39**, 697 (2007).

Received 28. 06. 2007