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Modeling of the Formation of Stress-Induced ω Phase in Metastable β Titanium Alloys

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Titanium alloys are materials with exceptional properties including high specific strength, extreme corrosion resistance, and biocompatibility. Among them, metastable β titanium alloys are a prospective group exhibiting complex phase transformations which can be employed to improve the performance of the material. Microstructural mechanisms controlling phase transformations in these alloys are not completely understood. In this work, we propose a continuum-based model describing non-diffusional, displacive, reversible $\beta \rightarrow \omega$ phase transformation which leads to a formation of stress-induced ω_{def} phase. The proposed model utilizes a well-developed mathematical theory of martensitic phase transitions based on the Cauchy–Born hypothesis, and reformulates this theory to describe the crystallographic mechanism of $\beta \rightarrow \omega_{\text{def}}$ phase transformation. The model evaluates compatibility criteria at the interfaces between β and ω_{def} phases in relation to the external stress and provides conditions for the formation of ω_{def} phase.

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1. Introduction

Titanium and titanium alloys have been attracting an increasing interest in the aerospace, automotive and chemical industries, deep-sea drilling, and medicine owing to their outstanding mechanical performance (e.g. high specific strength and fatigue resistance), exceptional corrosion resistance, and biocompatibility [1].

Titanium is an allotropic metal which undergoes a phase transformation from low temperature α phase (hcp) to high temperature β phase (bcc) at β-transit temperature $T_\beta = 882\,^\circ\text{C}$. In general, T_β is influenced by additions of alloying elements. Depending on the type and the amount of β stabilizing elements and the resulting phase composition at room temperature, titanium alloys are divided into α, $\alpha + \beta$, metastable β, and stable β alloys. Metastable β titanium alloys are versatile materials with regard to thermo-mechanical processing and resulting microstructure and mechanical properties [2, 3]. Therefore, the most in-depth research in the field of titanium alloys is focused on the development and characterization of metastable β alloys [4–6]. These alloys contain a sufficient amount of β stabilizing elements to suppress the martensitic transformation to α phase below room temperature. In this way, the bcc β phase is retained in a metastable state during quenching (from temperatures above T_β) and further undergoes several phase transformations involving different mechanisms [7].

Athermal metastable omega (ω_{ath}) phase is formed in various less-stabilized metastable β alloys during quenching [8, 9]. The ω_{ath} particles are finely distributed and their size is $\approx$ 1–2 nm [10, 11]. Upon annealing at temperatures in the range 300–400 °C, a fraction of athermal omega phase reverses back to the β phase and the remaining fraction evolves via diffusion processes to form isothermal omega phase ω_{iso} [12, 13]. Subsequent alpha precipitation (α_{nano}) occurrs at higher temperatures (400–600 °C) with the ω_{iso} particles acting as nucleation sites. Finally, upon annealing in the $\alpha + \beta$ field, stable $\alpha + \beta$ composition can be achieved. Another type of phases occurring in the metastable β alloys are the stress-induced ω_{def} and α'' phases [14, 15]. They typically form at very low strains and their formation was shown to be further affected by the content of β stabilizing elements [16] and oxygen [17].

Such wide variety of phases and phase transformations in metastable β titanium may open new possibilities of controlling the microstructure via optimized heat treatment and mechanical preloading. However, understanding of mechanisms underlying the evolution of these phases is rather incomplete.

A well-developed non-linear mathematical theory of displacive "shuffle" phase transitions exists and successfully accounts for the martensitic transformations in shape memory alloys [18]. The objective of this study is to reformulate such continuum-based theoretical model to explain the stress-induced diffusionless displacive $\beta \rightarrow \omega_{\text{def}}$ phase transformations in metastable β titanium alloys. Furthemore, the presented approach may be later utilized as a template for describing other phase transformations of this type.

2. Theory

This section briefly summarizes fundamental principles of the continuum mechanics theory, as presented in [18],

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which are employed in this work to formulate the theoretical model describing displacive $\beta \to \omega_{\mathrm{def}}$ phase transformations in metastable β titanium.

2.1. Continuum theory of deformation

Let $\boldsymbol{x}$ be a typical point (particle) in a body occupying a region Ω in three-dimensional space $\mathbb{R}^3$:

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \tag{1}$$

The deformation of this reference configuration is defined as a function $\boldsymbol{y} : \Omega \to \mathbb{R}^3$, where

$$\boldsymbol{y}(\boldsymbol{x}) = \begin{pmatrix} y_1(\boldsymbol{x}) \\ y_2(\boldsymbol{x}) \\ y_3(\boldsymbol{x}) \end{pmatrix} \tag{2}$$

is the position of the particle $\boldsymbol{x}$ in the new (deformed) configuration. The matrix of partial derivatives of deformation matrix $\boldsymbol{y}$, i.e. the matrix with components

$$\nabla(\boldsymbol{y})_{ij} = \frac{\partial y_i}{\partial x_j}, \quad i,j = 1,2,3 \tag{3}$$

is called the *deformation gradient* and for convenience is denoted $\boldsymbol{F}$, such that

$$\boldsymbol{F}(\boldsymbol{x}) = \nabla \boldsymbol{y}(\boldsymbol{x}). \tag{4}$$

Any homogeneous deformation can be then expressed as

$$\boldsymbol{y} = \boldsymbol{F}\boldsymbol{x} + \boldsymbol{c} \tag{5}$$

for some constant deformation gradient $\boldsymbol{F}$ and a constant translation vector $\boldsymbol{c}$.

Furthermore, it was shown in [18] that known deformation gradient can be used to calculate the strain in any direction according to the relation

$$\varepsilon_{\hat{\boldsymbol{e}}} = \sqrt{\hat{\boldsymbol{e}} \cdot (\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}\hat{\boldsymbol{e}})} - 1, \tag{6}$$

where $\varepsilon_{\hat{\boldsymbol{e}}}$ is the strain in the $\hat{\boldsymbol{e}}$ direction.

2.2. Kinematic compatibility condition

Let the solid body Ω be divided into two distinct parts Ω_1 and Ω_2 and apply different deformation gradients, $\boldsymbol{F}$ and $\boldsymbol{G}$, to the two parts, respectively

$$\boldsymbol{y} = \begin{cases} \boldsymbol{F}\boldsymbol{x} + \boldsymbol{c}, & \boldsymbol{x} \in \Omega_1, \\ \boldsymbol{G}\boldsymbol{x} + \boldsymbol{d}, & \boldsymbol{x} \in \Omega_2. \end{cases} \tag{7}$$

Consequently, the two parts of the body will be deformed in different ways. Should the deformation be continuous, the interface separating the two parts must remain coherent, i.e. it must undergo the same deformation from either deformation gradient. The equation

$$\boldsymbol{F} - \boldsymbol{G} = \boldsymbol{a} \otimes \hat{\boldsymbol{n}} \tag{8}$$

must be satisfied if the interface is to be coherent and the deformation continuous; where $\boldsymbol{a}$ is a shearing vector and $\hat{\boldsymbol{n}}$ is a reference normal of the interface. The equation is known as *kinematic compatibility condition* or *invariant plane condition*. In other words, any vector $\boldsymbol{v}$ lying on the interface is deformed by both deformation gradients, $\boldsymbol{F}$ and $\boldsymbol{G}$, equally

$$\boldsymbol{F}\boldsymbol{v} - \boldsymbol{G}\boldsymbol{v} = (\boldsymbol{a} \otimes \hat{\boldsymbol{n}})\boldsymbol{v} = 0 \quad \text{or} \quad \boldsymbol{F}\boldsymbol{v} = \boldsymbol{G}\boldsymbol{v}. \tag{9}$$

2.3. Continuum-based description of crystalline lattice. The Cauchy–Born hypothesis

The crystalline lattice can be linked to the continuum theory by employing the Cauchy–Born approximation [19]. The Cauchy–Born hypothesis says that the lattice vectors can be treated as infinitesimal line elements in the continuum. Consequently, if the solid undergoes some deformation $\boldsymbol{y}(\boldsymbol{x})$ (e.g. due to application of force) we can define a deformation gradient $\boldsymbol{F}(\boldsymbol{x})$ such as defined above. Crystalline lattice at the material point $\boldsymbol{x}$ after deformation will be distorted. If $\{\boldsymbol{e}'_i(\boldsymbol{x})\}$ are the lattice vectors of undistorted lattice, the lattice vectors of new (deformed) lattice $\{\boldsymbol{e}_i(\boldsymbol{x})\}$ are defined as

$$\boldsymbol{e}_i(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{x})\boldsymbol{e}'_i(\boldsymbol{x}). \tag{10}$$

Therefore, the Cauchy–Born hypothesis says that lattice vectors are deformed according to the applied deformation gradients. In other words, the positions of atoms within the crystal lattice follow the overall strain.

3. Formulation of the theoretical model

3.1. Geometrical description of the formation of ω_{def} phase

As mentioned above, the martensitic phase transformation leading to the formation of crystallographically different phase within the matrix of original phase is, in the framework of the theory of continuum mechanics combined with the Cauchy–Born hypothesis, described in terms of so-called deformation gradients. These gradients fully describe rearrangements of atoms (i.e. changes in the lattice parameters and/or the type of crystallographic structure) during the transformation.

The displacive $\beta \to \omega_{\mathrm{def}}$ transformation can be formally described as a collapse of two neighboring $(111)_\beta$ planes to their intermediate position, while the adjacent $(111)_\beta$ plane is left unchanged, the following two planes collapse again, and so forth [20] (see Fig. 1). In β titanium (bcc structure), the cubic cell structure can be regarded as the reference coordinate system, i.e. it is defined by vectors $[100]_\beta$, $[010]_\beta$, and $[001]_\beta$ in the Cartesian coordinate system. It can be shown that the cell of the hexagonal ω phase in the β reference frame is then defined by vectors $[1\bar{1}0]_\beta$, $[11\bar{2}]_\beta$, and $[111]_\beta$. Owing to the symmetry of this transformation, there is also a specific orientation relationship between the new ω_{def} lattice and the parent β phase

$$(0001)_\omega || (111)_\beta,$$

$$[11\bar{2}0]_\omega || [011]_\beta.$$

Since four sets of $(111)_\beta$ planes exist, there are four crystallographically equivalent realizations (variants) of the ω_{def} phase in the parent matrix.

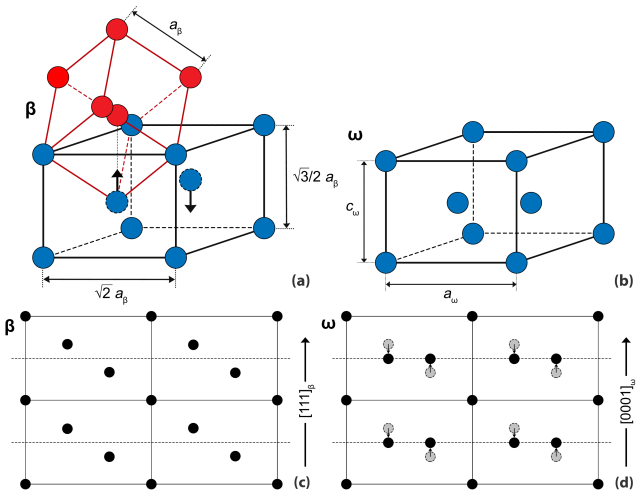

Fig. 1. Schematic view of displacive $\beta \rightarrow \omega_{\mathrm{def}}$ phase transformation in three dimensions: (a) β phase and (b) transformed ω_{def} phase; and in two dimensions (c) β phase and (d) transformed ω_{def} phase.

Geometrically, the lattice parameters of the newly formed ω_{def} phase (Fig. 1a) can be expressed as $a_\omega = \sqrt{2}a_\beta$ and $c_\omega = \frac{\sqrt{3}}{2}a_\beta$. However, owing to the displacement of the central atoms, the lattice parameters of the ω_{def} phase are slightly distorted and some misfit exists between the parameters obtained mathematically from the β phase and the parameters observed experimentally (Fig. 1b). Lattice parameters of the phases can be found in the literature; in this work, we consider $a_\beta = 3.28 \times 10^{-10}$ m, $a_\omega = 4.66 \times 10^{-10}$ m, and $c_\omega = 2.81 \times 10^{-10}$ m [21].

Taking into account the lattice parameters and the geometry of $\beta \rightarrow \omega_{\mathrm{def}}$ transformation, the four deformation gradients $\boldsymbol{F1}$ - $\boldsymbol{F4}$ completely describing the formation of ω_{def} phase variants can be easily determined. Let

$$m_1 = \frac{2}{\sqrt{3}}\frac{c_\omega}{a_\beta}, \quad m_2 = \frac{1}{\sqrt{2}}\frac{a_\omega}{a_\beta}$$

and

$$p_1 = \frac{m_1 + 2m_2}{3}, \qquad p_2 = \frac{m_1 - m_2}{3}.$$

Then, the deformation gradients are given by

$$\boldsymbol{F_1} = \begin{pmatrix} p_1 & p_2 & p_2 \\ p_2 & p_1 & p_2 \\ p_2 & p_2 & p_1 \end{pmatrix}, \qquad \boldsymbol{F_2} = \begin{pmatrix} p_1 & -p_2 & -p_2 \\ -p_2 & p_1 & p_2 \\ -p_2 & p_2 & p_1 \end{pmatrix},$$

$$\boldsymbol{F_3} = \begin{pmatrix} p_1 & p_2 & -p_2 \\ p_2 & p_1 & -p_2 \\ -p_2 & -p_2 & p_1 \end{pmatrix}, \quad \boldsymbol{F_4} = \begin{pmatrix} p_1 & -p_2 & p_2 \\ -p_2 & p_1 & -p_2 \\ p_2 & -p_2 & p_1 \end{pmatrix}.$$

3.2. Criteria for the ω_{def} phase formation

The fundamental principle of the proposed theoretical model is based on the solution of the set of Eqs. (11)–(14), which will be introduced here without comprehensive explanation. For derivations and further details on these equations see [18, 22].

Superscripts G denote variables related to the β phase, superscripts F are related to the ω_{def} phase.

$$\varepsilon_{kl}^F = S_{ijkl}^F \sigma_{ij}^F, \quad \varepsilon_{kl}^G = S_{ijkl}^G \sigma_{ij}^G, \tag{11}$$

$$\varepsilon_{kl}^F = \frac{\left(\boldsymbol{F}^{\mathrm{el}}\right)^{\mathrm{T}} \boldsymbol{F}^{\mathrm{el}} - \boldsymbol{I}}{2}, \quad \varepsilon_{kl}^G = \frac{\left(\boldsymbol{G}^{\mathrm{el}}\right)^{\mathrm{T}} \boldsymbol{G}^{\mathrm{el}} - \boldsymbol{I}}{2}, \tag{12}$$

$$\boldsymbol{Q}\left(\boldsymbol{F}^{\mathrm{el}}\right)^{\mathrm{T}} \boldsymbol{F} - \left(\boldsymbol{G}^{\mathrm{el}}\right)^{\mathrm{T}} \boldsymbol{G} = \boldsymbol{a} \otimes \hat{\boldsymbol{n}}, \tag{13}$$

$$\sigma_{ij}^F \hat{\boldsymbol{n}} = \sigma_{ij}^G \hat{\boldsymbol{n}}. \tag{14}$$

Equations (11) represent the Hooke law, i.e. the calculation of the second order tensor (third order square matrix) of elastic strain components ε_{kl} from the matrix of stress components σ_{ij} and the fourth order tensor of compliance constants, $\boldsymbol{S}_{ijkl}$ (inverse of the elastic constants tensor, $\boldsymbol{C}_{ijkl}$). Values of elastic constants for both phases are available in the literature [23, 24]. Equation (12) account for the calculation of tensors of elastic strain components ε_{kl}^F, ε_{kl}^G by means of elastic deformation gradients (atomic shifts caused by the elastic deformation), $\boldsymbol{F}^{\mathrm{el}}$ in the ω_{def} phase and $\boldsymbol{G}^{\mathrm{el}}$ in the β phase, $\boldsymbol{I}$ is the identity matrix.

Equation (13) is *the compatibility equation* and defines the criteria for the creation of $\beta/\omega_{\mathrm{def}}$ interface in the β phase, which may in turn lead to the formation of ω_{def} phase. $\boldsymbol{Q}$ is the rotation of the ω_{def} phase with respect to the β phase such that the continuity of the material is retained, $\boldsymbol{a}$ is the shearing vector at the interface between the atoms of the original β phase and the newly-developed ω_{def} phase, and $\hat{\boldsymbol{n}}$ is the interface normal. *Equilibrium equation* (14) finally ensures that stresses at the interface between the ω_{def} and β phase are in equilibrium.

4. Model algorithm

Solution of the system of equations is based on searching for an external stress $\sigma_{ij}^{\mathrm{ext}}$, such that all equations and specified criteria hold, i.e. the formation of the interface and, in turn, the ω_{def} phase itself is physically possible. The algorithm has been implemented using a *Matlab* software and *Optimization Toolbox* functions.

4.1. Rotation of the ω_{def} phase elastic constants

Before solving the actual equations, crystallographic properties of both phases must be taken into account. Due to geometric relation between the ω_{def} and β phase, the different reference coordinate systems must be considered when elastic constants need to be evaluated. The elastic constants of the ω_{def} phase in its orthogonal coordinate system $[1\bar{1}0]_\beta$, $[11\bar{2}]_\beta$, $[111]_\beta$ in the β reference frame must be unified with (i.e. "rotated" into) the primary reference coordinate system of the β phase $[100]_\beta$, $[010]_\beta$, $[001]_\beta$. For this purpose, a matrix of directional

cosines, A_{ij}, converting vectors from one coordinate system to the other, must be determined. The calculation of transformed elastic constants C^F_{ijkl} from the initial constants C^F_{mnrs} is then given by the relation

$$C^F_{ijkl} = A_{im}A_{jn}A_{kr}A_{ls}C^F_{mnrs}. \tag{15}$$

4.2. Model algorithm and the first results

The stress in the β phase, σ^{G}, is set to be equal to the external stress $\sigma^G = \sigma^{\mathrm{ext}}$ and is fixed as an input parameter. The objective is to find the stress in the ω_{def} phase, σ^F, in the form

$$\sigma^F = \boldsymbol{R}\sigma^F_{\mathrm{diag}}\boldsymbol{R}^{\mathrm{T}},$$

where σ^F_{diag} is a diagonal matrix and $\boldsymbol{R}$ is a general rotation. In this way, the physical nature of σ^F is maintained. Given the stresses in both phases, Eqs. (11) yield the strain matrices, ε^G_{kl} and ε^F_{kl}. In turn, these strain matrices enter into Eqs. (12) to give elastic deformation gradients, $\boldsymbol{G}^{\mathrm{el}}$ and $\boldsymbol{F}^{\mathrm{el}}$, in both β and ω_{def} phases, respectively.

Compatibility Eq. (13) requires elastic deformation gradients, $\boldsymbol{G}^{\mathrm{el}}$ and $\boldsymbol{F}^{\mathrm{el}}$, and deformation gradient of the omega phase, $\boldsymbol{F}$, (deformation gradient of the beta phase, $\boldsymbol{G}$, is obviously the identity matrix, $\boldsymbol{I}$) to be the inputs. The algorithm, which is analyzed in detail in [18], then calculates parameters $\boldsymbol{a}$, $\hat{\boldsymbol{n}}$, and $\boldsymbol{Q}$, whose meaning was defined in the previous sections. Furthermore, matrix $\boldsymbol{C}$, defined as:

$$\boldsymbol{C} = \left(\boldsymbol{G}^{\mathrm{el}}\boldsymbol{G}\right)^{-\mathrm{T}}\left(\boldsymbol{F}^{\mathrm{el}}\boldsymbol{F}\right)^{\mathrm{T}}\boldsymbol{F}^{\mathrm{el}}\boldsymbol{F}\left(\boldsymbol{G}^{\mathrm{el}}\boldsymbol{G}\right)^{-1} \tag{16}$$

and its eigenvalues can be determined. If the second eigenvalue, l_2, of the matrix $\boldsymbol{C}$ equals 1, "static" interface lying on an invariant plane can be formed between the phases. Finally, the equilibrium Eq. (14) must be satisfied in order to guarantee stress equilibrium at the interface.

Putting all this together, we are trying to find the stress in the ω_{def} phase, σ^F, such that the set of Eqs. (11)–(14) can be solved and it (i) satisfies the equilibrium Eq. (14) and (ii) gives the second eigenvalue, l_2, of the matrix $\boldsymbol{C}$ equal to 1. Therefore, we deal with a multi-objective optimization problem of 6 independent parameters (3 stress components and 3 Euler angles).

Given any stress σ^F and considering the matrix symmetries, the problem can be further simplified and the condition (ii) can be easily dealt with by an inverse recalculation of Eqs. (13)–(11) at each function evaluation/iteration

$$\boldsymbol{F}'^{\mathrm{el}} = \frac{\boldsymbol{F}^{\mathrm{el}}}{\sqrt{l_2}}, \tag{17}$$

$$\varepsilon'^F_{kl} = \frac{(\boldsymbol{F}'^{\mathrm{el}})^{\mathrm{T}}\boldsymbol{F}'^{\mathrm{el}} - \boldsymbol{I}}{2}, \tag{18}$$

$$\sigma'^F_{ij} = C^F_{ijkl}\varepsilon'^F_{kl}. \tag{19}$$

Consequently, σ'^F is the recalculated stress in the ω_{def} phase such that the second eigenvalue, l_2, of the matrix $\boldsymbol{C}$ equals 1. In this way, the optimization algorithm is simplified and becomes a single-objective optimization with the aim to minimize Eq. (14) in the form

$$||\sigma'^F_{ij}\hat{n} - \sigma^G_{ij}\hat{n}||. \tag{20}$$

In order to test the feasibility of the proposed model, four different uniaxial stresses σ^G in the β phase, 5, 10, 15, and 20 MPa, were fed into the model as an input. Minimization was carried out in the *Matlab Optimization toolbox*, using *fminsearch* algorithm. It should be noted that only the first variant of the ω_{def} phase, $\boldsymbol{F_1}$, was taken into account in these calculations.

Stresses σ'^F in the ω_{def} phase and parameters $\boldsymbol{a}$, $\hat{\boldsymbol{n}}$, and $\boldsymbol{Q}$ which satisfy the conditions for the formation of ω_{def} phase were successfully determined and are presented in Table I. Examination of the physical background of the parameters and comparison with the experimental data are the objectives of an ongoing work.

TABLE I

First results of the proposed model; uniaxial stresses σ^G of 5, 10, 15, and 20 MPa were fed into the optimization algorithm. Stresses σ'^F in the ω_{def} phase and other parameters were successfully calculated.

σ^G [MPa]	σ'^F [MPa]	$\hat{\boldsymbol{n}}$	$\boldsymbol{a}$	$\boldsymbol{Q}$
$\begin{pmatrix} 5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 4.06 & 1.44 & -0.72 \\ 1.44 & -4.14 & -0.42 \\ -0.72 & -0.42 & -1.76 \end{pmatrix}$	$\begin{pmatrix} 0.84 \\ 0.34 \\ -0.42 \end{pmatrix}$	$\begin{pmatrix} -0.06 \\ 0.04 \\ -0.06 \end{pmatrix}$	$\begin{pmatrix} 0.99 & -0.02 & 0.04 \\ 0.02 & 0.99 & 0.02 \\ -0.04 & -0.00 & 0.99 \end{pmatrix}$
$\begin{pmatrix} 10 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 8.19 & 2.75 & -1.94 \\ 2.75 & -8.98 & -0.66 \\ -1.94 & -0.66 & -4.81 \end{pmatrix}$	$\begin{pmatrix} 0.87 \\ 0.30 \\ -0.39 \end{pmatrix}$	$\begin{pmatrix} -0.11 \\ 0.07 \\ -0.10 \end{pmatrix}$	$\begin{pmatrix} 0.99 & -0.05 & 0.06 \\ 0.05 & 0.99 & 0.02 \\ -0.06 & -0.00 & 0.99 \end{pmatrix}$
$\begin{pmatrix} 15 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 15.30 & 0.19 & -0.65 \\ 0.19 & -11.99 & 11.29 \\ -0.65 & 11.29 & -9.89 \end{pmatrix}$	$\begin{pmatrix} 0.75 \\ 0.46 \\ 0.48 \end{pmatrix}$	$\begin{pmatrix} -0.17 \\ 0.11 \\ 0.10 \end{pmatrix}$	$\begin{pmatrix} 0.99 & -0.08 & 0.07 \\ 0.08 & 0.99 & 0.00 \\ 0.07 & -0.01 & 0.99 \end{pmatrix}$
$\begin{pmatrix} 20 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 19.31 & 3.73 & -2.78 \\ 3.73 & -26.53 & 6.77 \\ -2.78 & 6.77 & -21.65 \end{pmatrix}$	$\begin{pmatrix} 0.99 \\ 0.12 \\ -0.09 \end{pmatrix}$	$\begin{pmatrix} -0.12 \\ 0.07 \\ -0.08 \end{pmatrix}$	$\begin{pmatrix} 0.99 & -0.04 & 0.05 \\ 0.04 & 0.99 & 0.00 \\ -0.05 & -0.00 & 0.99 \end{pmatrix}$

5. Conclusions

The main results of this work can be summarized as follows:

- Vast variety of phases and phase transformations in metastable β titanium alloys make them suitable candidates for the systematic control of their microstructure and, in turn, mechanical properties.
- Theoretical model was formulated to describe the $\beta \rightarrow \omega_{\mathrm{def}}$ transformation occurring in metastable β Ti alloys.
- Conditions for the formation of stress-induced ω_{def} phase, i.e. stresses in the ω_{def} phase and additional parameters, were determined for given uniaxial stresses in the β phase. In this way, the theory of continuum mechanics combined with the Cauchy–Born hypothesis proved to be feasible to describe displacive phase transformations.
- The proposed model can be further developed and used as a template for designing "customized" models of this type of phase transformations also occuring in other materials.

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