MARTENSITE PHASE TRANSFORMATION MODEL TO PREVENT THE PSEUDOELASTIC PHENOMENON OF NITI ALLOY

Bo Zhou*

School of Applied Sciences, Harbin University of Science and Technology, Harbin, China.

E-mail: bozhou@gmail.com

Muhammad Ali Turgunov

Department of Mechanical and Aerospace Engineering, Turin Polytechnic University, Tashkent, Uzbekistan.

E-mail: m.turgunov@polito.uz

*Corresponding author

Abstract

A new phase transformation model is developed based on the basics of theorems about martensite phase transformation in solid materials. It is able to reflect the influences of phase transformation peak temperatures as well as the phase transformation start temperature and the phase transformation finish temperature, which overcomes the limitation that the previous phase transformation models can not reflect the influences of the phase transformation peak temperatures on the phase transformation behaviors of a NiTi alloy. Numerical examples illustrate the capability of the new phase transformation model. The thermo-mechanical behaviors of NiTi alloy are investigated through monotonic tensile tests. The multi-cycle mechanical behaviors and material training effects of NiTi alloy are investigated through multi-cycle tensile tests. A new phase transformation model with a material training effect is supposed to describe the multi-cycle phase transformation behaviors of NiTi alloy.

Keywords: martensite, NiTi, transformation model, superelasticity, shape memory

I. INTRODUCTION

A NiTi alloy is a special kind of metal with two unique thermo-mechanical phenomena. The shape memory effect is the phenomenon that the large material residual strain after loading and unloading can be fully recovered upon heating as shown in Figure 1. The pseudoelastic is the phenomenon that the large material strain upon loading can be fully recovered upon unloading as shown in Fig. 2. These special characteristics are due to the reversible change of solid crystal structures, which can be interpreted as the phase transformations in a NiTi alloy on changing material stress and temperature. Besides the shape memory effect and the superelasticity, a NiTi alloy usually possesses good biocompatibility, good corrosion, and excellent mechanical properties. For example, it can be used as actuators and sensor elements in aircraft structures due to the shape memory effect, as surgical treatment devices in medical applications due to superelasticity and biocompatibility, and as robotic muscles in automated structure due to superelasticity.

Tanaka [1] developed an exponent-type phase transformation model at first. Liang and Rogers [2] suggested a cosine-type phase transformation model based on the experimental study and Tanaka's model. Brinson [3] suggested another cosine-type model based on Liang's model describe the phase transformation behaviors below the martensite start temperature. There is no distinct difference between Liang's model and Brinson's model in mathematical nature. Ivshin and Pence [4] also developed a phase transformation model based on the fundamental thermodynamic consideration, which needs to formulate a relatively complex mathematical expression.

Only the influence of phase transformation starts and finish temperatures on the phase transformation behaviors is considered in previous phase transformation models.

In this research paper, a new phase transformation model is developed based on thermodynamics and martensitic phase transformation. It can reflect the influence of the phase transformation peak temperatures on the phase transformation behaviors as well as the influence of the phase transformation start and finish temperatures. The numerical calculations indicate the new phase transformation model can describe the phase transformation behaviors of NiTi alloy more precisely and effectively than the previous phase transformation models.

II. THEORETICAL BACKGROUND

2.1. Microscopic Explanation of Phase Transformation Behaviors

There exists one of three different microscopic structures in a NiTi alloy shown in Fig. 3. Fig. 3(a) is the austenite phase (B2), a structure of cubic lattices. Fig. 3(b) is the twinned martensite phase (B19), a structure of orthorhombic lattices. Fig. 3(c) is the detwinned martensite phase (B19'), a structure of monoclinic lattices. Both special macroscopic characteristics of the shape memory effect and the superelasticity are the results of the phase transformations among the austenite, the twinned martensite, and the detwinned martensite due to the change of stress or temperature.

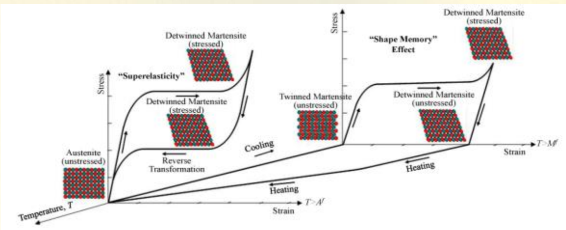


Figure 1 Shape memory effect of NiTi alloy

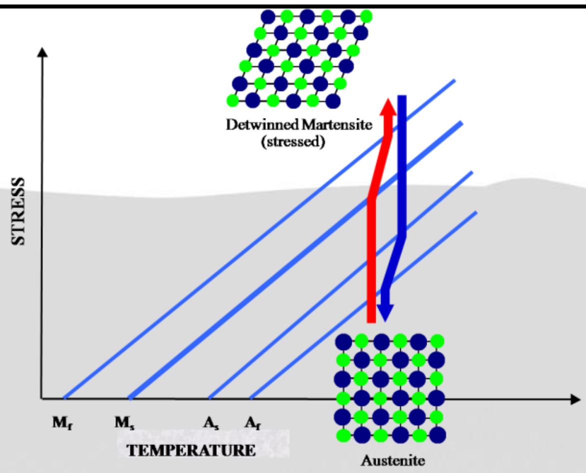


Figure 2 Pseudoelasticity of NiTi alloy

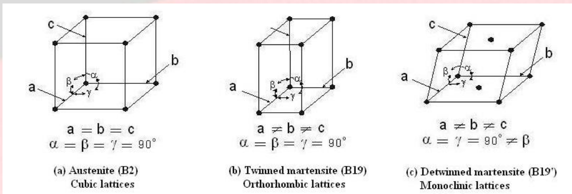


Figure 3 Different microcosmic structures in NiTi alloy

Fig. 4 illustrates the microscopic mechanism of the phase transformation in a NiTi alloy. Fig. 4(a) is the schematic diagram of the thermally induced phase transformation in NiTi alloys. Under stress-free conditions, there exists the austenite in the high-temperature state and the twinned martensite in the low-temperature state. The phase transformation from the martensite to the austenite takes place through the process of heating to the temperature above Af and the phase transformation from the austenite to twinned martensite takes place through the process of cooling to the temperature below Mf. Fig. 4(b) is the schematic diagram of the microscopic mechanisms of the phase transformations of the shape memory effect. During the loading, the material transforms from the austenite (or twinned martensite) phase to the detwinned martensite phase and obtains the large inelastic phase transformation strain. In a stress-free state, the material can transform from the detwinned martensite phase to the austenite phase and the material residual strain disappears completely through heating to the temperature above Af, expressing a shape memory effect.

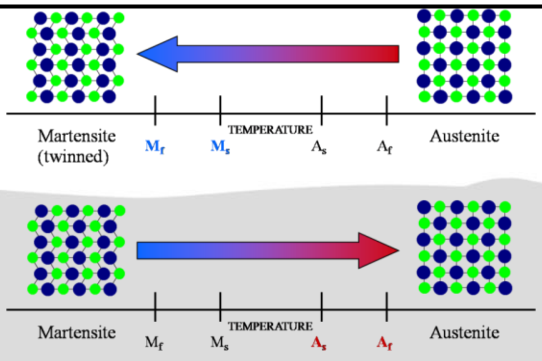


Figure 4(a). Thermally Induced Phase Transformation in NiTi alloys

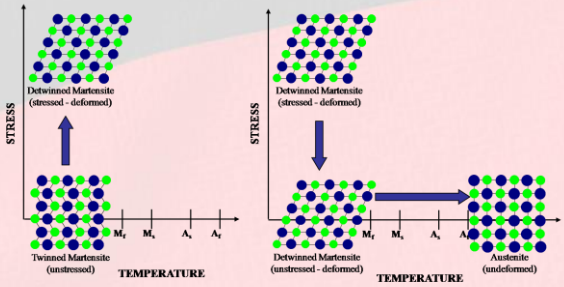


Figure 4(b) Microcosmic mechanisms of the phase transformations in NiTi alloy

III. RESULTS AND DISCUSSIONS

3.1. New Model

Fig. 5 shows the typical heat flow-temperature curve obtained from a DSC test. It is well known that the phase transformation behaviors of a NiTi alloy are influenced by the phase transformation peak temperatures as well as the phase transformation start and finish temperatures. While the influence of phase transformation peak temperatures on the phase transformation behaviors of a NiTi alloy is neglected by all previous phase transformation models. So, it is necessary to develop a new phase transformation model that can reflect the influence of the phase transformation peak temperatures on the phase transformation behaviors.

The value of the heat quantity needed by the phase transformation is expressed by ΔQ which equals the area of the curvilinear triangle MsMpMf during the phase transformation from the austenite to the martensite or AsApAf during the phase transformation from the martensite to the austenite. The function of the heat-temperature curve segment MsMpMf during the phase transformation from the austenite to the martensite or AsApAf during the phase transformation from the martensite to the austenite is defined by f(T), so there is the following differential relation between f(T) and ΔQ.

$$f(T) = \frac{d\Delta Q}{dT} \qquad (1)$$

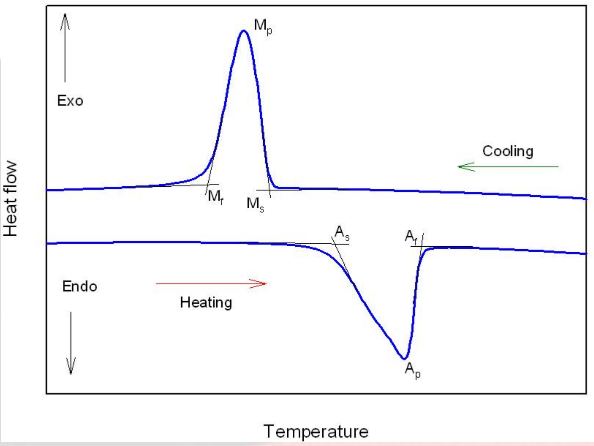


Figure 5 Heat flow-temperature curves of DSC test

According to Fig. 2, the heat-temperature curve segments *AsAp* and *ApAf* during the phase transformation from the martensite to the austenite can be assumed as the triangle functions

$$f(T) = A\sin\left(\frac{T - A_s}{a_1}\right) + C_1 \qquad (A_p > T > A_s) \tag{2a}$$

and

$$f(T) = A\cos\left(\frac{T - A_p}{a_2}\right) + C_1 \qquad (A_f > T > A_p) \tag{2b}$$

where

$$a_1 = \frac{2(A_p - A_s)}{\pi} \tag{2c}$$

and

$$a_2 = \frac{2(A_f - A_p)}{\pi} \tag{2d}$$

Substituting Equation (1) into Equations (2a) and (2b) leads to

$$\frac{d\Delta Q}{dT} = A\sin\left(\frac{T - A_s}{a_1}\right) + C_1 \qquad (A_p > T > A_s) \tag{3a}$$

and

$$\frac{d\Delta Q}{dT} = A\cos\left(\frac{T - A_p}{a_2}\right) + C_1 \qquad (A_f > T > A_p) \tag{3b}$$

Similarly, the heat-temperature curve segments *MsMp* and *MpMf* during the phase transformation from the austenite to the martensite can be assumed as the triangle functions

$$f(T) = B\sin\left(\frac{T - M_s}{m_1}\right) + D_1 \qquad (M_p < T < M_s) \tag{4a}$$

and

$$f(T) = B\cos\left(\frac{T - M_p}{m_1}\right) + D_1 \qquad (M_f < T < M_p) \tag{4b}$$

where

$$m_1 = \frac{2(M_p - M_s)}{\pi} \tag{4c}$$

and

$$m_2 = \frac{2(M_f - M_p)}{\pi} \tag{4d}$$

Substituting Equation (1) into Equations (4a) and (4b) leads to

$$\frac{d\Delta Q}{dT} = B\sin\left(\frac{T - M_s}{m_1}\right) + D_1 \qquad (M_p < T < M_s) \tag{5a}$$

and

$$\frac{d\Delta Q}{dT} = B\sin\left(\frac{T - M_p}{m_1}\right) + D_1 \qquad (M_f < T < M_p) \tag{5b}$$

During the phase transformation, the free energy increment is denoted by ΔG, the heat energy increment is denoted by ΔQ and the entropy increment is denoted by ΔS. According to thermodynamics, the following differential relationship should be satisfied between the free energy increment ΔG, the heat energy increment ΔQ, and the entropy increment ΔS.

$$\frac{d\Delta G}{dT} = \frac{d\Delta Q}{dT} - \Delta S \tag{6}$$

According to the martensite phase transformation, there should be the following differential relationship between the martensitic volume fraction ξ and the free energy increment ΔG during the phase transformation.

$$\frac{d\xi}{dT} = k\frac{d\Delta G}{dT} + C_2 \tag{7}$$

Substituting Equation (6) into Equation (7) leads to

$$\frac{d\xi}{dT} = k\frac{d\Delta Q}{dT} + C_3 \tag{8}$$

where $C_3 = C_2 - k\Delta S$.

If both derivatives of martensitic volume fraction ξ with respect to temperature T at the austenite start temperature and the austenite finish temperature are assumed to be zero, i.e.

$$\frac{d\xi}{dT} = 0 \qquad (T = A_s \quad or \quad T = A_f)$$

The relationship between the martensitic volume fraction ξ and the temperature T during the phase transformation from the martensite to the austenite can be simply expressed as the equations

$$\frac{d\xi}{dT} = kA\sin\left(\frac{T - A_s}{a_1}\right) \qquad (A_p > T > A_s) \tag{9a}$$

and

$$\frac{d\xi}{dT} = kA\cos\left(\frac{T - A_p}{a_1}\right) \qquad (A_f > T > A_p) \tag{9b}$$

from Equations (3) and (8).

Integrating equation (9a) for the range of $A_p > T > A_s$ with the boundary condition of $\xi(A_s) = 1$ and Equation (9b) for the range of $A_f > T > A_p$ with the boundary condition of $\xi(A_f) = 0$ and using the condition that both values of $\xi(A_p)$ from Equation (9a) and (9b) should be the same, one can obtain the equations

$$\xi = \frac{a_1}{a_1 + a_2}\cos(\frac{T - A_s}{a_1}) + \frac{a_2}{a_1 + a_2} \qquad (A_p > T > A_s) \tag{10a}$$

and

$$\xi = -\frac{a_2}{a_1 + a_2}\sin(\frac{T - A_p}{a_2}) + \frac{a_2}{a_1 + a_2} \qquad (A_f > T > A_p) \tag{10b}$$

Equations (10a) and (10b) are the functions describing the relationship between the martensitic volume fraction ξ and temperature T during the phase transformation from the martensite to the austenite in the stress-free state.

In a similar manner, if both derivatives of the martensitic volume fraction ξ with respect to temperature T at martensite start temperature and martensite finish temperature are assumed to be zero, i.e.

$$\frac{d\xi}{dT} = 0 \qquad (T = M_s \quad or \quad T = M_f)$$

The relationship between the martensitic volume fraction ξ and the temperature T during the phase transformation from the austenite to the martensite can be simplify expressed as the equations

$$\frac{d\xi}{dT} = kB\sin\left(\frac{T - M_s}{m_1}\right) \qquad (M_p < T < M_s) \tag{11a}$$

and

$$\frac{d\xi}{dT} = kB\cos\left(\frac{T - M_p}{m_2}\right) \qquad (M_f < T < M_p) \tag{11b}$$

from Equation (5) and (8).

Integrating Equation (11a) for the range of $M_p < T < M_s$ with the boundary condition of $\xi(M_s) = 0$ and Equation (11b) for the range of $M_f < T < M_s$ with the boundary condition of $\xi(M_f) = 1$ and using the condition that both values of $\xi(M_p)$ from Equations (11a) and (11b) should be the same, one can obtain the equations.

$$\xi = -\frac{m_1}{m_1 + m_2}\cos\left(\frac{T - M_s}{m_1}\right) + \frac{m_1}{m_1 + m_2} \qquad (M_p < T < M_s) \tag{12a}$$

and

$$\xi = \frac{m_2}{m_1 + m_2}\sin\left(\frac{T - M_p}{m_2}\right) + \frac{m_1}{m_1 + m_2} \qquad (M_f < T < M_p) \tag{12b}$$

Equations (12a) and (12b) are the functions describing the relationship between the martensitic volume fraction ξ and the temperature T during the phase transformation from the austenite to the martensite in the stress-free state.

As mentioned before, M_s, M_p and M_f are the martensite start temperature, the martensite peak temperature and the martensite finish temperature in the stress-free state during the phase transformation from the austenite to the martensite, respectively. A_s, A_p, and A_f are the austenite start temperature, the austenite peak temperature and the austenite finish temperature in the stress-free state during the phase transformation from the martensite to the austenite, respectively. If the martensite start temperature, the martensite peak temperature and the martensite finish temperature in the stressed state during the phase transformation from the austenite to the martensite are expressed by M_s^σ, M_p^σ and M_f^σ, respectively. The austenite start temperature, the austenite peak temperature, and the austenite finish temperature in the stressed state during the phase transformation from the martensite to the austenite are expressed by A_s^σ, A_p^σ, and A_f^σ, respectively.

Using the relationship between phase transformation critical stresses and temperature in Fig. 6 leads to the following relationships.

$$M_s^\sigma = \frac{\sigma}{C_M} + M_s \tag{13a}$$

$$M_p^\sigma = \frac{\sigma}{C_M} + M_p \tag{13b}$$

$$M_f^\sigma = \frac{\sigma}{C_M} + M_f \tag{13c}$$

and

$$A_s^{\sigma} = \frac{\sigma}{C_A} + A_s \qquad (13e)$$

$$A_p^{\sigma} = \frac{\sigma}{C_A} + A_p \qquad (13f)$$

$$A_f^{\sigma} = \frac{\sigma}{C_A} + A_f \qquad (13g)$$

Replacing *As*, *Ap* and *Af* in Equations (2,c~d) and (10,a~b) with A_s^{σ}, A_p^{σ}, and A_f^{σ} in Equations (10,a~c), one can have the equations describing the function relationships between martensitic volume fraction ξ, temperature T and material stress σ during the phase transformation from the martensite to the austenite as

$$\xi = \frac{a_1}{a_1 + a_2}\cos(\frac{T - A_s^{\sigma}}{a_1}) + \frac{a_2}{a_1 + a_2} \quad (A_p^{\sigma} > T > A_s^{\sigma}) \qquad (14a)$$

and

$$\xi = -\frac{a_2}{a_1 + a_2}\sin(\frac{T - A_p^{\sigma}}{a_2}) + \frac{a_2}{a_1 + a_2} \quad (A_f^{\sigma} > T > A_p^{\sigma}) \qquad (14b)$$

Replacing *Ms, Mp* and *Mf* in Equations (4,c~d)) and (12,a~b) with M_s^{σ}, M_p^{σ} and M_f^{σ} in Equations (13,d~g), one can have the equations describing the function relationships between martensitic volume fraction ξ, temperature T and material stress σ during the phase transformation from the austenite to the martensite as

$$\xi = -\frac{m_1}{m_1 + m_2}\cos(\frac{T - M_s^{\sigma}}{m_1}) + \frac{m_1}{m_1 + m_2} \quad (M_p^{\sigma} < T < M_s^{\sigma}) \qquad (14c)$$

and

$$\xi = \frac{m_2}{m_1 + m_2}\sin(\frac{T - M_p^{\sigma}}{m_2}) + \frac{m_1}{m_1 + m_2} \quad (M_f^{\sigma} < T < M_p^{\sigma}) \qquad (14d)$$

Equation (14) is the new phase transformation model describing the phase transformation behaviors of a NiTi alloy where the coefficients a1, a2, m1 and m2 are shown in Equations (2c), (2d), (4c) and (4d), respectively. Using the new phase transformation model, Equation (14), and the constitutive law with constant material functions, Equation (3), one can also describe the mechanical behaviors of a NiTi alloy.

It is different from the previous models, in that the new phase transformation model can reflect the influence of phase transformation peak temperatures as well as the phase transformation start and finish temperatures on the phase transformation behaviors of a NiTi alloy. This makes up the limitation that the previous model cannot reflect the influence of phase transformation peak temperatures on the phase transformation behaviors, so the new phase transformation model can predict the phase transformation behaviors more precisely and effectively than the previous models.

IV. NUMERICAL SIMULATIONS

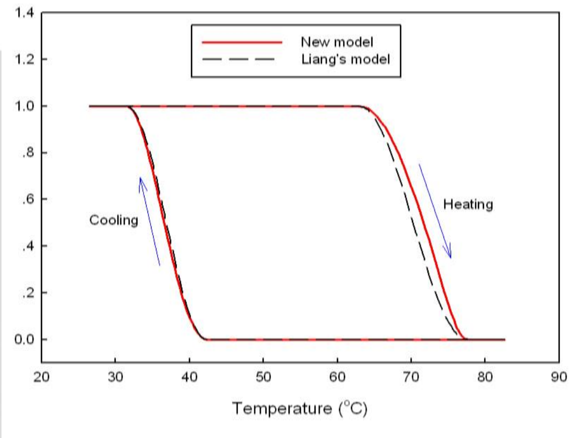
The numerical simulation calculations and the phase transformation temperatures are taken from the previous experimental results of the DSC test and they are listed in Table 1. The relational coefficients of CM and CA are taken as 8.0MPa/□C and 13.8MPa/□C, respectively.

Fig. 8 and Fig. 9 show martensitic volume fraction-temperature curves described by the new phase transformation model, Equation (14), compared with Liang's phase transformation model and Tanaka's phase transformation model.

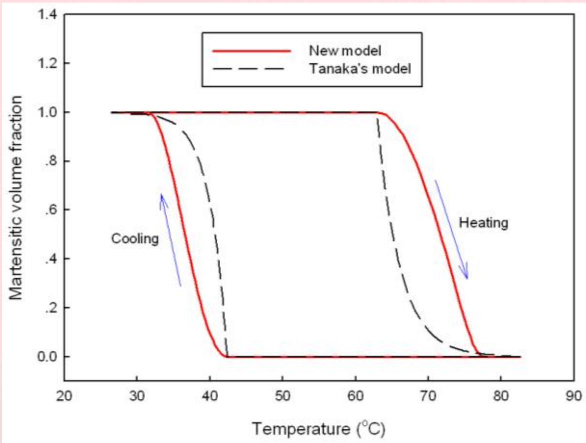
Table I PHASE TRANSFORMATION TEMPERATURE OF NITI ALLOY

Annealing temperature (ºC)	Mf (ºC)	Mp (ºC)	Ms (ºC)	As (ºC)	Ap (ºC)	Af (ºC)
600	31.42	36.03	42.36	62.88	74.22	77.64
900	33.54	40.00	44.74	60.05	73.85	77.30

Equation (1), respectively, the annealing temperatures for Fig. 6 and Fig. 7 are 600oC and 900oC, respectively. Fig. 6(a) and Fig. 7(a) show the cases of the comparison between the new phase transformation model and Liang's phase transformation model. Fig. 6(b) and Fig. 7(b) show the cases of the comparison between the new phase transformation model and Tanaka's phase transformation model. The results of Liang's model and Tanaka's reveal that the shape of the curve during the phase transformation from the austenitic NiTi alloy phase to the martensitic phase is the same as that during the phase transformation from the martensitic phase to the austenitic NiTi alloy phase. However, the results of the new phase transformation model reveal that the shape of the curve during the phase transformation from the austenitic NiTi alloy c phase to the martensitic phase is different from that during the phase transformation from the martensitic phase to the austenitic NiTi alloy phase. Therefore, it is known that the new phase transformation model can describe the phase transformation behaviors of a NiTi alloy more precisely than Liang's model and Tanaka's model, especially in the case with the unsymmetrical heat-temperature curves. From the comparison of the new model with the previous models, the difference between the new model and Tanaka's model is bigger than that between the new model and Liang's model. This is because that both Liang's model and the new model possess the mathematical expression of trigonometric function while Tanaka's model possesses the mathematical expression of exponent function.

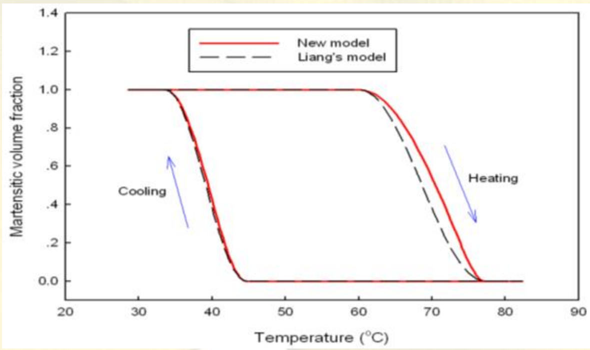


(a) Comparison with Liang's model

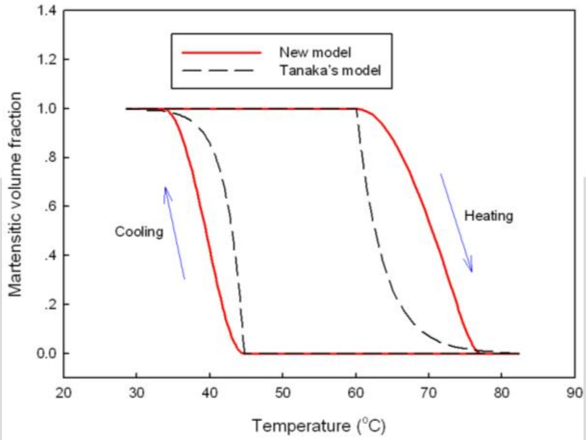


(b) Comparison with Tanaka's model

Fig. 6 Martensitic volume fraction-temperature curves with annealing 600oC



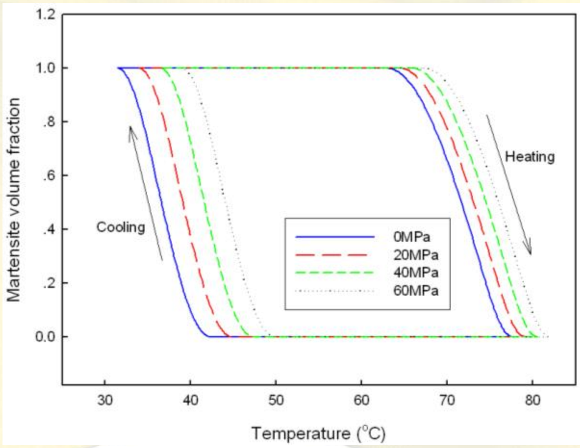
(a) Comparison with Liang's model



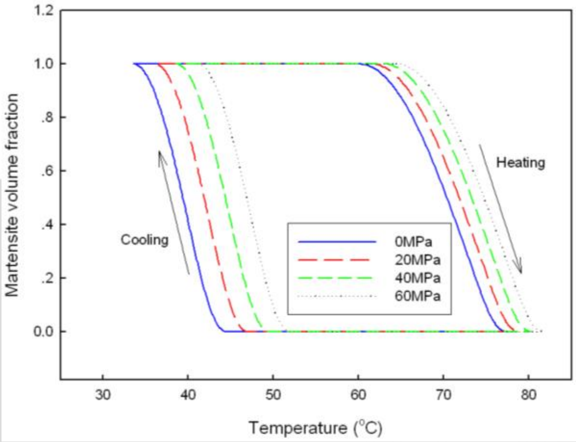
(b) Comparison with Tanaka's model

Fig. 7 Martensitic volume fraction-temperature curves with annealed 900oC

Fig. 8 shows the martensitic volume fraction-temperature curves described by the new phase transformation model, Equation (14), with different constant material stresses which include 10MPa, 20MPa, 40MPa, and 60MPa. Fig. 7(a) is the martensitic volume fraction-temperature curves at the case of annealing 600□C and Fig. 7(b) is the martensitic volume fraction-temperature curves at the case of at 900□C. According to the results, the phase transformation temperatures tend to increase as the stress level increases which accords with the relationship between phase transformation critical stress and temperature shown as in Fig. 6. The increment extent in the martensitic volume fraction with respect to temperature under the phase transformation from the austenite to the martensite is larger than that under the phase transformation from the martensite to the austenite. Such result can be observed because the value of material constant CA (13.8MPa/oC) is higher than that of material constant CM (8MPa/oC).



(a) At case of annealed 600oC



(b) At case of annealed 900oC

Figure 8 Martensitic volume fraction-temperature curves with different stress state

V. CONCLUSION

The microscopic mechanism of phase transformation and the special behaviors of shape memory effect and superelasticity are introduced in detail. A new phase transformation model is developed based on the previous experimental results of a DSC test. The new phase transformation model takes the influence of phase transformation peak temperatures as well as the phase transformation start and finish temperatures. This makes up the limitation that the previous phase transformation models can not reflect the important influence of phase transformation start temperatures on the phase transformation behaviors of a NiTi alloy. The new phase transformation model, Tanaka's phase transformation model, and Liang's phase transformation model are used to predict the phase transformation behaviors of a NiTi alloy. They are also be used to describe the mechanical behaviors of a NiTi alloy together with the constitutive law with constant material functions. The comparison of numerical results between the new phase transformation model and the previous phase transformation models illustrates the capability of the new phase transformation model.

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