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Limitations of Constitutive Relations for TiNi Shape Memory Alloys

W. Tang and R. Sandström

Dept. of Materials Science and Engineering, Royal Institute of Technology, 100 44 Stockholm, Sweden

Abstract. Phase transformation tensor Ω in the constitutive equation proposed by Tanaka has been evaluated by employing experimental data of TiNi alloys in a constrained recovery process. It demonstrates that the absolute value of Ω for the constrained recovery process is typically about 0.6 ~ 0.7 x10^3 MPa, which is much smaller than that for the stress - induced martensitic transformation (typically 2.5 ~ 3.5 x10^3). Based on the evaluated results for Ω, predicted recovery stress - temperature relations by the constitutive equation are compared with the experimental data for TiNi rods under different strains. Big discrepancy exists for large strain conditions. Several transformation kinetic expressions are examined for the constitutive relation of the constrained recovery process.

1. INTRODUCTION

A significant amount of practical uses have been exploited for TiNi and Cu-based shape memory alloys (SMAs) [1, 2], in which SMAs are introduced as substitutes of traditional materials or provide entirely new designs due to the unique functions. As a smart material, design with SMA not only requires many unique properties, e.g. switch temperature, recovery stress, and stress rate, but also relies on the relationships among various property descriptors under thermomechanical routines. Tanaka [3-5] first applied continuum mechanics with an internal variable to describe the thermomechanical behaviour of SMA and formulated a unified constitutive relation which consists of the mechanical constitutive equation and the transformation kinetics. Later, Liang and Rogers [6,7] extended Tanaka's model to describe the stress-strain-temperature relations corresponding to different recovery processes such as the free recovery, the constrained recovery, and the controlled recovery. In comparison with others' work, Tanaka's model is easier to employ in engineering design and computation. However, according to our previous work [8], one of the material parameters involved in the constitutive equation, the phase transformation tensor Ω, has a strong influence on the quantitative description of the stress - strain - temperature relations of SMA. In the present work, more experimental data of TiNi alloys are employed to evaluate the transformation tensor Ω for the constrained recovery process. Moreover, different functions describing the transformation kinetics are going to be examined on the basis of the evaluated transformation tensor Ω.

2. EVALUATION OF THE TRANSFORMATION TENSOR Ω

According to Tanaka's model [3-5], the uniaxial thermomechanical behaviour of SMA is governed by the constitutive equation:

$$\sigma - \sigma_0 = D(\varepsilon - \varepsilon_0) + \Theta(T - T_0) + \Omega(\xi - \xi_0) \qquad (2.1)$$

here σ, ε and T are the state variables representing stress, strain and temperature, respectively. ξ is an internal variable as a function of σ and T, which measures the extent of the phase transformation.

$$\xi = \xi(\sigma, T) \qquad 0 \le \xi \le 1 \qquad (2.2)$$

(σ_0, ε_0, T_0, ξ_0) denotes the initial state. The material parameters D, Θ and Ω in Eq.(2.1) are the elastic modulus, the thermoelastic tensor and the transformation tensor, respectively.

To gain a better understanding of the material parameters in the constitutive relation, we rewrite Eq.(2.1) as

$$\Delta\varepsilon = \frac{\Delta\sigma}{D} - \frac{\Theta}{D}\Delta T - \frac{\Omega}{D}\Delta\xi \qquad (2.3)$$

where $\Delta\varepsilon$ is the total strain change which consists of three terms: (1) the linear elastic strain change $\Delta\varepsilon_{lin} = \Delta\sigma/D$, (2) the thermal expansion term $\Delta\varepsilon_{th} = -(\Theta/D)\Delta T$, and (3) the strain change caused by phase transformation $\Delta\varepsilon_{tr} = -(\Omega/D)\Delta\xi$.

The transformation tensor Ω is a metallurgical quantity which reflects the crystallographic volume change during phase transformation. Comparing with the two other parameters D and Θ, there is no direct approach to measure Ω [6]. Based on Eq.(2.3), the transformation tensor Ω can be expressed as

$$\Omega = -D\Delta\varepsilon_{tr}/\Delta\xi \qquad (2.4)$$

which can be regarded as the basic equation for evaluating Ω. According to Eq.(2.4), Ω must be a negative parameter since the martensitic transformation in non-ferrous SMA always leads to a volume expansion.

Fig.1 demonstrates the schematic stress-temperature (σ-T) relation during the constrained recovery process. From T_0 to A_s^1 (the reverse transition starting temperature under stress), there is no reverse transition occurring. We get the constitutive equation in this temperature range as

$$\sigma = \Theta' (T - T_0) \qquad T_0 \leq T \leq A_s^1 \qquad (2.5)$$

here Θ' value can be obtained by measuring the slope of the initial stage of the σ-T recovery curve. The reason why Θ' (>0) instead of the thermoelastic tensor Θ (<0) is employed has been stated in our previous work [8]. Experimental results show that the slope of the σ-T recovery curve in the initial stage is always positive, whereas the thermoelastic tensor Θ is negative according to Eq.(2.3). Consequently, the parameter Θ' is introduced in order to reflect the effects from thermal expansion and other factors such as the internal stress.

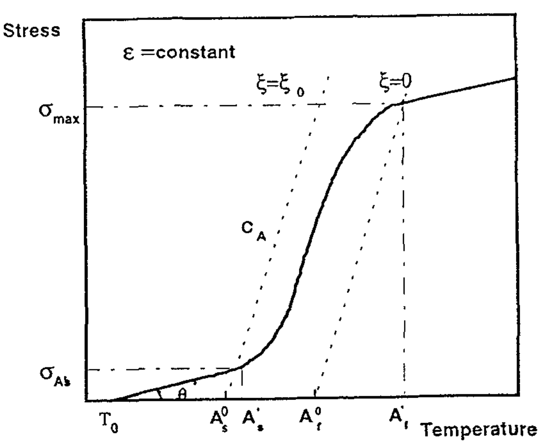

Fig.1 Schematic stress-temperature relation during constrained recovery for a TiNi SMA.

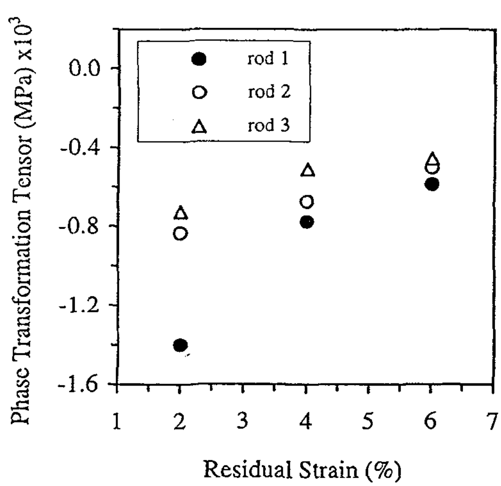

Fig.2 Relation between phase transformation tensor and residual strain for three TiNi rods.

The transformation zone is between the dashed lines $\xi = \xi_0$ and $\xi = 0$, and the constrained reverse transition starts form A_s^1 to A_f^1 (the reverse transformation finishing temperature under stress). The recovery stress at

A_f^1 is referred to as the maximum recovery stress σ_{max}. Within the temperature range from A_s^1 to A_f^1, the constitutive equation becomes

$$\sigma = \Theta'(T - A_s^1) + \Omega(T)(\xi - \xi_0) + \sigma_{A_s^1} \quad (2.6)$$

Now we start from Eq.(2.4) to evaluate Ω for TiNi alloys by applying experimental data from the constrained martensitic reverse transformation. For the constrained recovery, we have

$$\Delta\varepsilon_{tr} = \Delta\varepsilon_{total} - \Delta\varepsilon_{lin} - \Delta\varepsilon_{th}$$
$$= 0 - \Delta\sigma/D + (\Theta'/D)\Delta T \quad (2.7)$$

thus Eq.(2.4) becomes

$$\Omega(T) = \frac{\sigma - \sigma_{A_s^1} - \Theta'(T - A_s^1)}{\xi - \xi_0} \quad (2.8)$$

Ω at $T = A_f^1$ and $\sigma = \sigma_{max}$ can be calculated without knowing $\xi(\sigma, T)$ function as:

$$\Omega = -\frac{\sigma_{max} - \sigma_{A_s^1} - \Theta'(A_f^1 - A_s^1)}{\xi_0} \quad (2.9)$$

where $\xi_0 = \varepsilon_r / \varepsilon_L$.

Table 1 presents the initial transformation temperatures (stress free) and compositions for three TiNi rods. The corresponding experimental data of the constrained recovery process are shown in Table 2, which are from a company data sheet [9]. The three TiNi rods have undergone the same thermomechanical treatment. They were deformed in tension at temperature T_0 below A_s, and unloaded with the residual strain ε_r equal to 2%, 4% and 6%, respectively. Then they were heated by keeping the residual strain constant.

Table 1 Compositions and transformation temperatures for three TiNi rods [9]

	Ni (at%)	M_s^0	M_f^0	A_s^0	A_f^0 (°C)
Rod 1	50.49	4	-12	7	23
Rod 2	50.19	32	18	48	69
Rod 3	49.95	72	48	83	106

Table 2 Experimental data of constrained recovery for the above three TiNi rods

	ε_r (%)	ε_L (%)	A_s' (°C)	A_f' (°C)	T_0 (°C)	Θ' (MPa/°C)	C_A (MPa/°C)	$\sigma_{A_s'}$ (MPa)	$\sigma_{A_f'}$ (MPa)	b_A (1/MPa) $\times 10^{-3}$
Rod 1	2	6	8	96	-16	0.30	6.82	6.82	501	9.16
	4	6	8	104	-16	0.30	6.82	6.82	554	9.16
	6	6	8	115	-16	0.30	6.82	6.82	626	9.16
Rod 2	2	6	49	110	25	0.30	7.38	7.38	304	6.45
	4	6	49	134	25	0.30	7.38	7.38	483	6.45
	6	6	49	142	25	0.30	7.38	7.38	539	6.45
Rod 3	2	6	84	144	60	0.30	6.96	6.96	267	6.25
	4	6	84	159	60	0.30	6.96	6.96	369	6.25
	6	6	84	176	60	0.30	6.96	6.96	490	6.25

By applying experimental data in Table 2 to Eq.(2.9), the transformation tensor Ω at (σ_{max}, A_f^1) is obtained for the three TiNi rods as shown in Fig.2. Results in Fig.2 indicate that the absolute value of Ω for the constrained recovery process (typically 0.5 ~ 0.7x10^3 MPa) is much smaller in comparison with that for the stress-induced martensitic transformation (typically 2.5 ~ 3.5x10^3 MPa). For the same TiNi rod, the $|\Omega|$ value decreases with increasing the residual strain. Fig.2 also shows that, Ω data are more scattered at small residual strain and tend to converge around -0.6x10^3MPa at larger residual strain. Generally speaking, Ω is not very sensitive to M_s temperature or to alloy composition.

Assessment of Ω by employing experimental data from the NASA reports [10, 11] further proves that the $|\Omega|$ value for the constrained recovery process is typically around 0.6 ~ 0.8 x10^3 MPa. The results are in a very good agreement with the results indicated in Fig.2.

3. COMPARISON BETWEEN EXPERIMENTAL AND PREDICTED σ - T RELATIONS

We assume that Ω doesn't change with the temperature during the whole constrained recovery process and takes the value at A_f^1 since this value is irrelevant to the selection of $\xi(\sigma, T)$ describing the transformation kinetics. Then based on Eq.(2.6) the recovery stress - temperature (σ - T) relation can be derived by choosing proper $\xi(\sigma, T)$ expressions.

According to the experimental phenomenology, the martensite fraction $\xi = \xi(\sigma, T)$ in the reverse transformation can be expressed as exponential, sine, cosine or linear function of $x = b_A C_A (T - A_s^0) - b_A \sigma$ with boundary conditions as follows [8]

$$\xi = \exp[(-2\ln 10)x] \qquad \xi(0) = 1, \xi(1) = 0.01^* \qquad (3.1)$$

$$\xi = 1 - \sin[90x] \qquad \xi(0) = 1, \xi(1) = 0 \qquad (3.2)$$

$$\xi = 0.5\cos[180x] + 0.5 \qquad \xi(0) = 1, \xi(1) = 0 \qquad (3.3)$$

$$\xi = 1 - x \qquad \xi(0) = 1, \xi(1) = 0 \qquad (3.4)$$

By using Eq.(2.6) together with Eqs.(3.1) ~ (3.4), relations between the recovery stress and temperature (σ-T) can be deduced by employing the initial conditions and the material parameters presented in Table 1 and 2. To solve these equations and derive σ-T relation, iteration method has to be applied. Representative calculations are demonstrated in Figs.3 ~5 for TiNi Rod 2 together with the experimental data. It has been found that the predicted σ-T relations are in a good agreement with the experimental data when the residual strain is 2%, whereas bigger discrepancy exists for 4% and 6% strain tests. It indicates that this constitutive relation is not suitable for quantitatively describing σ-T relation under large residual strains. It has also been observed that, among all $\xi(\sigma, T)$ expressions, cosine function, provides the σ-T relation that is closest to the experimental data no matter the alloy composition and the amount of residual strain.

Based on the results above, we can say that it is acceptable to assume that Ω is constant during the constrained recovery process and take the value at (σ_{max}, A_f^1). The discrepancy between the prediction and the experimental results is not likely to be dependent on the $\xi(x)$ expression since each $\xi(x)$ gives the similar tendency of σ - T curve, as shown in Figs.3 ~ 5, although cosine function produces the result closest to the experimental data. The problem could be in the expression of the intermediate variant $x = b_A C_A (T - A_s^0) - b_A \sigma$, which assumes that σ and T has equivalent effect on the transformation and the stress rate $d\sigma/dT$ is a constant C_A. This may result in a distance between the real martensite fraction and the empirical $\xi(\sigma, T)$ expressions at certain temperature. The question is to find a best x expression to minimise this distance.

If we input the experimental (σ, T) data of rod 2 into the constitutive Eq.(2.6), the martensite fraction can be deduced as shown in solid symbol for 4% strain in Fig.6, whereas the martensite fraction calculated by different empirical $\xi(\sigma, T)$ models, e.g. sine, cosine and exponential functions, is indicated as empty symbol in Fig.6, respectively. It shows that, the martensite fraction deduced from the constitutive relation decreases gradually with temperature, in contrast with the results calculated by the different $\xi(\sigma, T)$ models, which show an abrupt decrease at the beginning of the constrained recovery process. Traditionally, martensitic transformation is usually expressed as the exponential function [13, 14]. However, the transformation

* Here the austenite fraction is assumed to be 0.99 as usually done in metallurgy [12].

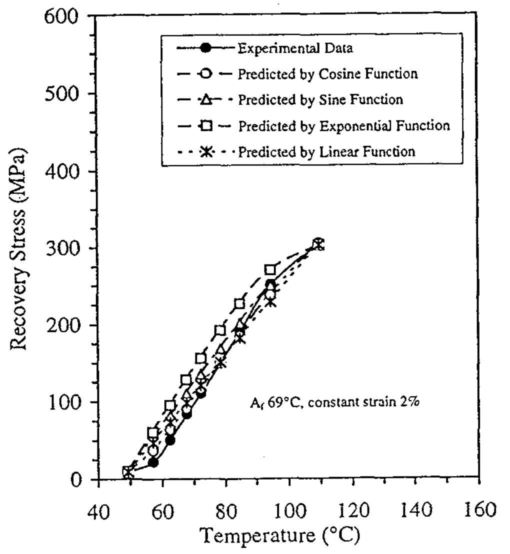

Fig.3 Comparison of experimental recovery stress-temperature data with predicted results for TiNi Rod 2 under 2% residual strain.

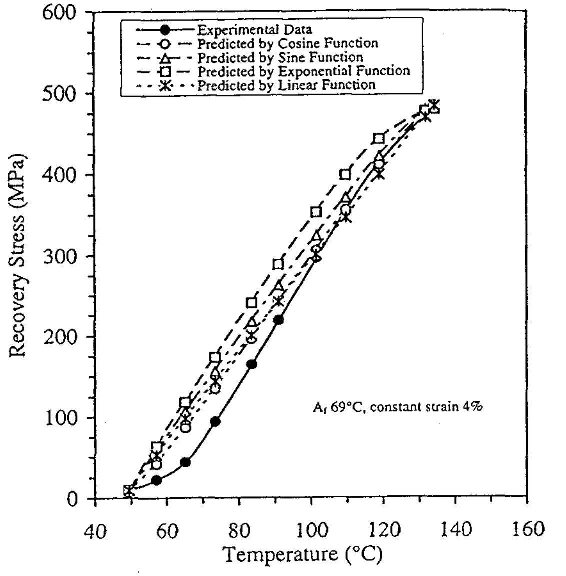

Fig.4 Comparison of experimental recovery stress-temperature data with predicted results for TiNi rod 2 under 4% residual strain.

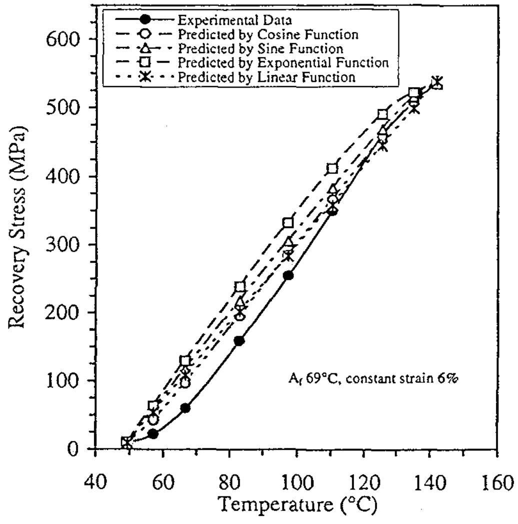

Fig.5 Comparison of experimental recovery stress-temperature data with predicted results for TiNi Rod 2 under 6% residual strain.

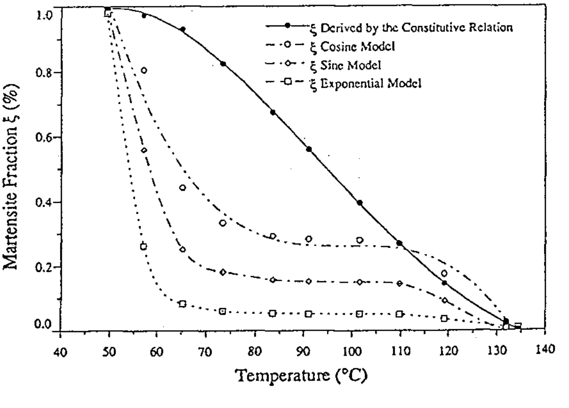

Fig.6 Relation between martensitic fraction and temperature during the constrained recovery process for TiNi rod 2 with 4% constant strain.

involved here is a special one — a constrained recovery process. With the strain being kept from restoring, its transformation kinetics could be different, and it is reasonable that the reverse transformation proceeds gradually with temperature due to the recovery constraint. Fig.4 implies that the strength of σ should be increased in $x = b_A C_A (T - A_s^0) - b_A \sigma$. Therefore, a new model for the transformation kinetics is needed for the constrained reverse transformation, in order to achieve a better prediction of constitutive relations.

4. CONCLUSIONS

Phase transformation tensor Ω in the constitutive relation for SMA has been evaluated by using experimental data of TiNi alloys for the constrained reverse martensitic transformation. It demonstrates that the absolute value of Ω (typically 0.6 ~ 0.7x10^3 MPa) is much smaller than that for the stress-induced martensitic transformation (typically 2.5 ~ 3.5x10^3 MPa). It means that one has to specify Ω for each transformation processes. For the same TiNi alloy, $|\Omega|$ value decreases with the increase of the residual strain. Comparison between the predicted recovery stress - temperature relations by the constitutive equation and the experimental data for TiNi rods under different residual strains shows that the constitutive equation is acceptable to describe the thermomechanical behaviour of TiNi rods with smaller strain, e.g. 2% in the present work. However, for larger strain conditions, big discrepancy indicates the limitations on using the constitutive equation. This may result from that $x = b_A C_A (T - A_s^0) - b_A \sigma$ is not suitable for the constrained recovery transformation. The transformation kinetics as well as the mechanical constitutive relation need to be studied further.

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