Study on Dynamic Constitutive Model and Parameter Analysis of Ti/Ni Shape Memory Alloy Based on Irreversible Thermodynamics

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Abstract. The dynamic constitutive model of Ti/Ni shape memory alloy based on irreversible thermodynamics theory was established by introducing two internal variables to characterize phase transformation and plastic deformation process. The evolution laws of phase transformation and plastic deformation were deduced respectively by assuming two generalized force associated with the corresponding internal variables.Latin Hypercube Sampling method is applied to sample among the whole parameter space for constitutive parameter of Ti/Ni alloy dynamic constitutive model based on irreversible thermodynamics theory, and Spearman rank correlation analysis of non-parameter statistics method is employed to conduct correlation analysis for random-input sample set of constitutive parameter and the output set of its corresponding objective function. A model is built to solve parameter sensitivity based on Spearman rank correlation coefficient, in order to achieve overall analysis of parameter sensitivity. According to results, numerical results, obtained with this method, are well consistent with experimental data. Furthermore, the optimal solution to the dynamic constitutive parameters can be realized with high efficiency, accuracy and reliability via the research method on parameter sensitivity analysis and identification put forward in this paper.

1. Introduction

Ti/Ni alloy is not only widely used in Aviation & Aerospace, Mechanics, Electronics, Energy, and Medical field [1-2], but also the Ti/Ni alloy high strain dynamic responding behavior is closely related to a great many of applications [3]. Meanwhile, the unique Shape Memory Effect and excellent Super-elasticity of the Ti/Ni alloy draws wide attention to researchers at home and abroad, and it is currently one of the Shape Memory Alloys that studied and applied most [4]. The Super elasticity of Ti/Ni alloy refers to the phenomenon that the strain, which produced under effect of external force, is far greater than its elastic limit, but self recovers when unloaded. The Shape Memory Effect refers to the phenomenon when material going through plastic deform, and being

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heated until certain temperature level is reached, it could restore the shape before deform [5]. zone, such that the fundamental frame of Super elasticity constitutive relations of Memory Alloy is built.

In order to study and apply the super elasticity and Shape Memory Effect of Ti/Ni alloy, a reasonable description of Ti/Ni alloy constitutive relation model is indeed necessary. Earlier phenomenological theory model proposed by Tanaka [6] is limited to one-dimension only. Liang C [7] expand its one-dimension constitutive model to three dimension. But neither of the above two model take the effect of temperature onMartensitic transformation into consideration, so the Martensitic reverse transformation cannot be described. Later in the model raised by Brinson[8], Martensitic transformation was divided into two parts, temperature induced transformation and stress induced transformation, therefore, Martensitic transformation dynamics equation has two evolution equation, positive and negative, under different temperature zone, such that the fundamental frame of Super elasticity constitutive relations of Memory Alloy is built.

Based on irreversible thermodynamics, a macro-phenomenological constitutive model is developed to describe the dynamic response of Ti/Ni alloy by introducing two internal variables to characterize phase transformation and plastic deformation evolution. Then this paper adopts Latin Hyper-cube Sampling method to sample among the whole parameter space of material parameter in Ti/Ni alloy dynamic constitutive model based on irreversible thermodynamics theory, adopts Spearman correlation analysis in non-parameter statistic method to conduct correlation analysis on randomly input sample set of constitutive parameter and the output set of corresponding objective function, to build an equation which adopts Spearman rank correlation coefficient to get equivalent solution of parameter sensitivity, in order to achieve overall analysis of parameter sensitivity. Based on the result obtained through Spearman rank correlation analysis, generic algorithm is applied to identify material parameter of Ti/Ni alloy dynamic constitutive model.

2. Ti/Ni alloy constitutive parameter identification model and constitutive parameter sensitivity analysis and generic algorithm procedure

Based on irreversible thermodynamics theory, Ti/Ni alloy dynamic constitutive model is defined[9], which contains eighteen parameters waiting to be identified. Based on its property, the model can be divided into four phases and optimize: Austenite elastic phase, transformation phase, Martensite elastic phase and plastic flow phase. Use the four vector below to represent the to-be-identified parameter of dynamic constitutive model in the four phases:

Austenite elastic phase:

$$X_A = [E_A]^T \tag{1}$$

Transformation phase:

$$X_{TR} = [z_1, n_1, k_1, k_2, s_{s0}^{tr}, c_1, c_2, s_{f0}^{tr}]^T \tag{2}$$

Martensite elastic phase:

$$X_M = [E_M]^T \tag{3}$$

Plastic flow phase:

$$X_P = [z_2, n_2, k_3, k_4, s_{y0}^{p}, c_3, m, R_1]^T \tag{4}$$

The purpose of Ti/Ni alloy constitutive parameter identification is to find out the optimal value of X^* in four phases, to achieve the minimum result of the equation of (5) of each phase.

$$W(X^*) = \min \sqrt{\sum_{i=1}^{n} (\sigma(\varepsilon_i) - \sigma_i)^2} \tag{5}$$

Since Ti/Ni alloy constitutive model is non-linear, and subject to the mutual effect of numerous parameters, the correlation analysis among random variables is conducted using non-parameter statistic method, using Spearman rank correlation coefficient to measure the correlation among random variables. Before conducting overall analysis on parameter sensitivity, it is necessary to apply Latin Hypercube Sampling method (LHS) [10] to sample in the whole range of Ti/Ni alloy constitutive parameters. And sensitivity degree r_i of parameter x_i, which can be expressed as below:

$$r_i = \left| \frac{n\sum_{k=1}^{n}\alpha_k\beta_k - \sum_{k=1}^{n}\alpha_k\sum_{k=1}^{n}\beta_k}{\sqrt{n\sum_{k=1}^{n}(\alpha_k)^2 - (\sum_{k=1}^{n}\alpha_k)^2}\sqrt{n\sum_{k=1}^{n}(\beta_k)^2 - (\sum_{k=1}^{n}\beta_k)^2}} \right| \tag{6}$$

Generic algorithm is an algorithm which mimics natural biological evolution mechanism. Through encoding initial group, operate based on their adaptability to environment, and achieve survival of the fittest evolutionary process. Generic algorithm is composed of three basic generic operators: Selection, Crossover, and Mutation.

3. Ti/Ni alloy constitutive parameter identification

This paper uses Split Hopkinson Pressure Bar (SHPB) device in dynamic mechanics laboratory of SiChuan University, to test dynamic compressive performance of Ti/Ni alloy.

3.1. Solution of Ti/Ni alloy dynamic constitutive parameter sensitivity

Ti/Ni alloy dynamic constitutive parameter and the LHS range of each parameter are shown as Table 1. 20 times of unit sampling is conducted within the range of each parameter. Based on the Spearman Rank definition method from previous section, the rank value of Ti/Ni alloy dynamic constitutive parameter can be obtained, as shown in Table 2. According to equation (6), Spearman correlation coefficient of Ti/Ni alloy dynamic constitutive parameter can be calculated, as shown in Table 3. From the calculated result, it can be confirmed that the sensitivity degree value of z_1 Z_2 n_1 n_2 c_1 c_2 c_3 σ_{s0}^{tr} σ_{f0}^{tr} σ_{y0}^{p} R_1 E_M E_A is fairly large, which means the effect of parameter on output value is fairly large, and whose value should be focused on while identifying Ti/Ni alloy dynamic constitutive parameter. However, sensitivity value of k_1, k_2, k_3, k_4 is rather small, which means these parameter has less effect on output value during calculation, and be considered as sub-influencing factor of Ti/Ni alloy dynamic constitutive.

Based on Spearman rank correlation analysis theory, to make sure the accuracy of generic algorithm, it is necessary to adjust the range and sampling times of each parameter, in order to make sensitivity degree value of each parameter close to each other and all less than 0.2.

Table 1. Dynamic constitutive parameters of Ti/Ni alloy.

E_A / MPa	E_M / MPa	Z_1 / MPa	n_1	k_2	k_1	σ_{s0}^{tr}/MPa	c_1	c_2
10^5~$4x10^5$	10^5~$3x10^5$	0-15	0~10	500~900	200~500	200~500	0~1	0~1
uniformity	uniformity	uniformity	uniformity	uniformity	uniformity	uniformity	uniformity	uniformity
σ_{f0}^{tr} / MPa	Z_2 / MPa	n_2	k_4	k_3	σ_{y0}^{p} / MPa	c_3	m	R_1
200~500	0~200	0~10	600~900	200~500	500~2000	0~0.1	100~300	0~100
uniformity	uniformity	uniformity	uniformity	uniformity	uniformity	uniformity	uniformity	uniformity

Table 2. Rank of Latin hypercube sampling data.

z_1	n_1	k_2	k_1	σ_{s0}^{tr}	c_1	c_2	σ_{f0}^{tr}	z_2	n_2	k_4	k_3	σ_{y0}^{p}	c_3	m	R_1	E_A	E_M
16	11	7	17	16	15	4	9	16	11	9	7	4	2	17	16	16	11
19	3	14	4	15	6	14	12	19	3	10	14	8	12	4	15	19	3
6	9	15	9	20	9	8	17	6	9	19	15	15	8	9	20	6	9
11	8	10	3	14	17	16	18	11	8	4	10	6	13	3	14	11	8
15	13	5	20	4	16	15	4	15	13	2	5	12	15	20	4	15	13
5	10	1	19	6	18	13	11	5	10	13	1	14	1	19	6	5	10
8	5	20	6	19	14	18	16	8	5	6	20	20	19	6	19	8	5
14	1	3	12	8	13	3	15	14	1	17	3	7	14	12	8	14	1
17	15	6	10	18	7	20	14	17	15	18	6	16	5	10	18	17	15
1	2	17	7	3	3	11	3	1	2	8	17	10	20	7	3	1	2
3	14	8	5	10	1	2	6	3	14	1	8	19	3	5	10	3	14
7	18	2	18	9	2	9	13	7	18	5	2	18	17	18	9	7	18
20	6	13	13	2	10	12	1	20	6	16	13	17	4	13	2	20	6
18	12	16	14	11	19	5	5	18	12	11	16	3	9	14	11	18	12
4	16	9	8	13	11	19	20	4	16	12	9	2	10	8	13	4	16
9	17	18	11	5	8	1	19	9	17	15	18	11	6	11	5	9	17
13	7	19	16	12	12	17	7	13	7	3	19	1	18	16	12	13	7
2	20	12	2	7	4	7	10	2	20	14	12	13	7	2	7	2	20
12	19	4	15	1	20	10	8	12	19	20	4	5	11	15	1	12	19
10	4	11	1	17	5	6	2	10	4	7	11	9	16	1	17	10	4

Table 3. Dynamic constitutive parameter sensitivity of Ti/ Ni alloy.

E_A / MPa	E_M / MPa	Z_1 / MPa	n_1	k_2	k_1	σ_{s0}^{tr} /MPa	c_1	c_2
0.225	0.27	0.242	0.26	0.085	0.018	0.269	0.21	0.2375
σ_{f0}^{tr} / MPa	Z_2 / MPa	n_2	k_4	k_3	σ_{y0}^{p} / MPa	c_3	m	R_1
0.355	0.24	0.261	0.005	0.013	0.72	0.269	0.02	0.269

3.2. Generic algorithm optimization of Ti/Ni Alloy dynamic constitutive parameter

Based on irreversible thermodynamics theory, Ti/Ni alloy dynamics constitutive model can be created. During identification of constitutive parameter using generic algorithm, this constitutive model can be divided into four phases: parent elastic phase, transformation phase, Marstensite elastic phase and plastic flow phase, build objective function on 4 phases respectively. Table 4. is the range of parameters in generic algorithm. Next, based on the range of all above mentioned parameter, use generic algorithm to conduct identification and solving for each parameters. During solving, set crossover rate as 0.5, mutation rate as 0.09, number of generation as 500, binary digit for each variable is 9.Finally Ti/Ni alloy dynamic constitutive parameter can be obtained, as shown in Table 5.

Substitute the optimal solution of above mentioned parameters into Ti/Ni alloy dynamic constitutive correlation, based on the characteristics of master equation of Ti/Ni alloy constitutive correlation, semi-implicit stress integration method is applied, which is to solve non-elastic strain increment amount using semi-implicit iteration method, and update explicit equation at next incremental step to get point (ε, σ). On this basis, the incremental format describing phase deformation plasticity process of the Ti/Ni alloy is derived. In addition, nonlinear iterative algorithms is raised and the calculation program composed in Fortran language to constructively demonstrate the impact process under different strain rates. Refer to Figure 1 for details.

Table 4. Parameter range.

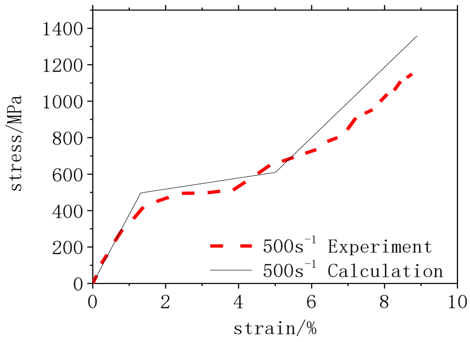
E_A / MPa	E_M / MPa	Z_1 / MPa	n_1	k_2	k_1	σ_{s0}^{tr} /MPa	c_1	c_2
10^5~4×10^5	10^5~2×10^5	0~15	0~10	500~900	200~500	400~500	0~1	0~1
σ_{f0}^{tr} / MPa	Z_2 / MPa	n_2	k_4	k_3	σ_{y0}^{p} / MPa	c_3	m	R_1
350~600	0~200	0~10	700~900	300~500	1000~2000	0~0.0001	200~300	0~100

Table 5. Optimal solution of dynamic constitutive parameters of Ti/Ni alloy.

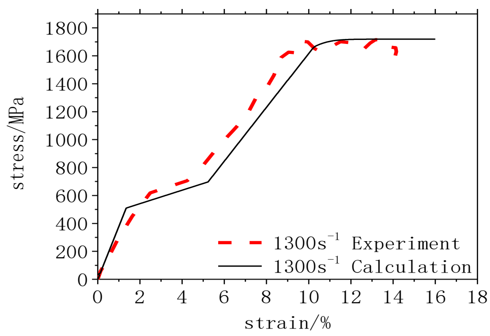
E_A / MPa	E_M / MPa	Z_1 / MPa	n_1	k_2	k_1	σ_{s0}^{tr} /MPa	c_1	c_2
37807	19288	10.87	3.0098	797.16	410.14	400	0.0378	0
σ_{f0}^{tr} / MPa	Z_2 / MPa	n_2	k_4	k_3	σ_{y0}^{p} / MPa	c_3	m	R_1
556.36	172.3	4	806	401.9	1464.1	0	256.7	49.2

Based on optimal solution of Ti/Ni alloy dynamic constitutive parameter in Table 5. stress-strain numerical simulation result of Ti/Ni alloy under strain rate of $500s^{-1}$, $1300s^{-1}$, $1500s^{-1}$, $2100s^{-1}$, $3000s^{-1}$ can be obtained, and comparison with experimental result is shown as Figure 1. From the calculated result, numerical result of Ti/Ni alloy dynamic constitutive model matches nicely with experimental value. Under these five strain rate, Ti /Ni alloy dynamic constitutive curve during the whole simulation process shows 4 phases: Austenite elastic phase, transformation phase, Martensitic elastic phase, plastic flow phase, indicates the sensitivity of Ti /Ni alloy dynamic constitutive coefficient can be achieved using Spearman rank correlation analysis, and Ti /Ni alloy dynamic constitutive parameter identification can be achieved using generic algorithm. The simulation results are higher than experimental data after dislocation plastic deformation occurs and the deviations increase obviously with the increasing strain rate. This phenomenon might result in the following reasons proposed by Zeng et al[9]. The plastic deformation of materials under a high strain rates is regarded as an adiabatic process so that the heat produced by plastic work cannot dissipate in time. And its dynamic stress-strain response is an essentially coupled result of strain-rate strengthening, strain hardening and adiabatic softening effects. The temperature in material rises will cause the decrease in the initial yield stress, which is the so-called adiabatic softening effect.

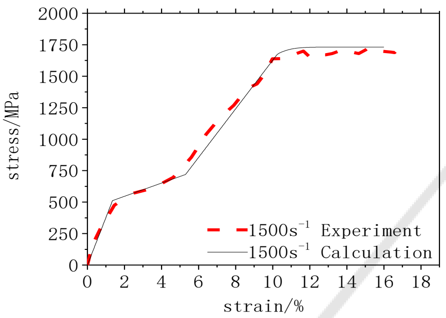
At the same time, overall analysis of parameter sensitivity and generic algorithm in this paper has important reference meaning to the identification of other engineering materials.



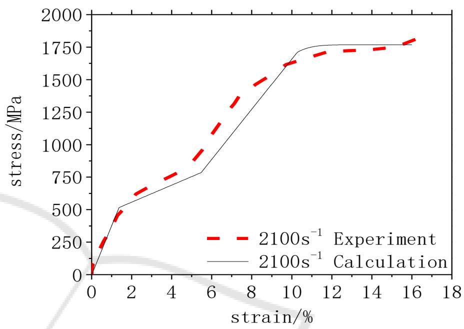
(a)The loading strain rate is $500s^{-1}$



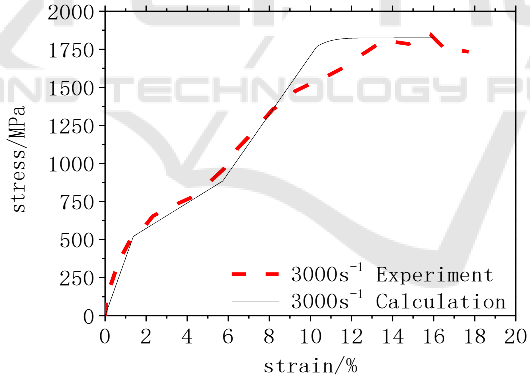
(b) The loading strain rate is $1300s^{-1}$



(c)The loading strain rate is $1500s^{-1}$



(d) The loading strain rate is $2100s^{-1}$



(e) The loading strain rate is$3000s^{-1}$

Figure 1. Stress and strain curves for Ti/Ni alloy at different strain rate.

4. Conclusions

Applied Super-Latin Cube Sampling method to sample among the whole parameter space, and used Spearman rank correlation analysis in non-parameter statistic method to conduct correlation analysis on random input sample set of constitutive parameter and its corresponding objective function output, hence achieved overall analysis of parameter sensitivity. Based on Spearman rank correlation coefficient, it reflected the impact extent of Spearman correlation coefficient on objective function of Ti/Ni alloy dynamic constitutive parameter, and then confirmed the primary-secondary relation among each parameter, and provided an effective method for multi-factor systematic analysis. This method overcomed shortcomings of single-factor analysis, so it is a more practical method.Sensitivity value of Ti/Ni alloy dynamic constitutive parameter, obtained through Spearman rank correlation analysis, defined the range of constitutive parameter. Generic algorithm was used to identify Ti/Ni alloy dynamic constitutive parameter, making the workload of identifying constitutive model parameter much less heavy, and locating the optimal solution in a fast, accurate and reliable manner.

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References

[1] Elahinia M H, Hashemi M, Tabesh M and Bhaduri S B 2012 Functionally graded Ni-Ti microstructures synthesised in process by direct laser metal deposition *J. Prog. Mater.Sci.* 57 911
[2] Es-Souni M, Es-Souni M and Fischer-Brandies H 2005 Biointerface: protein enhanced stem cells binding to implant surface *J. Anal. Bioanal.Chem.* 381 557
[3] Millett J C F, Bourne N K and GrayIII G T 2002 High strain-rate, small strain response of a NiTi shape-memory-alloy *J. Appl. Phys.* 92 3107
[4] Wang X M, Yue Z F, Wang Y F and et al 2009 *Superelastic mechanical properties of NiTi alloy and its application* M. Beijing: Science Press
[5] Yang J and Wu Y H 1993 *Shape memory alloy and its application* M. Hefei University of Science and Technology China press
[6] Tanaka K A 1986 Thermomechanical sketch of shape memoryeffect: One-dimension tensile behavior *J.Res.Mechanica* (18) 251-263
[7] Liang C and Rogers C A 1990 One-dimension thermomechanical constitutive relation for shape memory alloy *J. J.of Intell.Mater.Syst. and Struct* (1) 207-234
[8] Brinson L C and Lammering R 1993 Finite-element analysis of thebehavior of shape-memory alloys and their applications *J. International Journal of Solids and Structures* **30(23)** 3261-3280
[9] Chen H Y, Chen C, Zeng X G, Chen J and Guo Y 2016 Nified onstitutive odel for hase ransformation and lastic ehavior of Shape Memory Alloy Based on the irreversible thermodynamics *J.journal of sichuan university (engineering science edition)* **48(2)** 219-224
[10] Simpson T W, Lin D K J, Chen W 2001 Sampling strategiesb for computer experiments: Design and analysis *J.International Journal of Reliability and Applications* **2(3)** 209-240