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Simulation of isothermal reversible strain in the $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy using a microstructural model

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Recently it has been found that some NiTi-based alloys may undergo the forward martensite transition on isothermal holding. Moreover, such isothermal transformation under stress is accompanied by variation in reversible strain. At the same time, theoretical models do not allow describing the recoverable strain variation during holding. The aim of the present study was to adjust the microstructural model earlier developed by V. Likhachev and A. Volkov for describing strain variation due to the formation of the martensite phase on holding of NiTi-based alloys under a constant stress at temperatures within the temperature range of the forward martensite transformation. To take into account the possibility for isothermal martensite formation, a new suggestion was made, according to which the isothermal kinetics might be controlled by some relaxation process, which could change the local density of point defects and led to the fulfillment of thermodynamics condition for transformation. To include this assumption into the model some modifications have been added to constitutive equations. The modified microstructural model was used to simulate the strain variation, caused by isothermal martensite formation under various stresses. The influence of holding parameters (temperature and stress) on the maximum isothermal strain was found, and a good agreement between the simulated and experimental results was obtained. It was shown that the modified microstructural model allowed predicting the holding temperature and the stress at which the maximum isothermal strain can be found.

Keywords: NiTi-based alloys, martensite transformations, isothermal holding, microstructural model.

УДК: 536.65

Моделирование изотермической обратимой деформации в сплаве $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ с помощью микроструктурной модели

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К настоящему времени обнаружено, что в ряде сплавов на основе TiNi прямое мартенситное превращение может происходить в условиях изотермической выдержки. Более того, под нагрузкой такое превращение сопровождается изменением обратимой деформации. Однако, изменение деформации при изотермической выдержке под нагрузкой не может быть описано с помощью существующих теоретических моделей. В связи с этим целью настоящей работы явилось модификация микроструктурной модели, разработанной ранее В. Лихачевым и А. Волковым, для описания изменения обратимой деформации, обусловленного формированием мартенсита при выдержке сплавов на основе TiNi под постоянной нагрузкой при температурах внутри температурного интервала прямого мартенситного перехода. Для того чтобы учесть возможность изотермического образования мартенсита, было предположено, что изотермическая кинетика превращения может контролироваться некоторым релаксационным процессом, который приводит к локальному изменению плотности дефектов, что приводит к выполнению условия прямого превращения. Чтобы учесть сделанное предположение, были внесены изменения в определяющие соотношения модели. Используя модифицированную модель, было проведено моделирование изменения деформации в процессе изотермических выдержек при разных температурах под различными нагрузками. Определено влияние параметров выдержки (температуры и напряжения) на максимальную величину изотермической деформации и показано, что расчетные данные хорошо согласуются с экспериментальными. Показано, что модифицированная модель позволяет предсказать температуру выдержки и величину приложенного напряжения, при которых наблюдается максимальная изотермическая деформация.

Ключевые слова: сплавы на основе TiNi, мартенситные превращения, изотермическая выдержка, микроструктурная модель.

1. Introduction

Recently, it has been shown that some NiTi-based shape memory alloys undergo the forward martensitic transformation during holding at a constant temperature close to M_s (start temperature of the forward martensitic transition) [1–7]. The kinetics of this process is well studied experimentally, and it is established that the martensite volume fraction increases with time up to a saturation value, which depends on the holding temperature in a non-monotonic way [5–7]. In [8–10], it was first shown that the realization of the isothermal martensite transformation under a constant stress is accompanied by the strain accumulation and that all this strain is returned on subsequent heating during the reverse transformation.

To simulate the isothermal formation of martensite in NiTi-based alloys in the stress-free state, several theoretical models have been suggested [1–3,10], but all of them are not focused on the calculation of the strain variation during the isothermal transformation. The strain variation during isothermal holding of the NiTi alloy under stress was simulated in [11]. However, holding of the sample was carried out at temperatures at which the alloy was in the fully martensite state. In this case, the strain variation could not be realized by the isothermal transformation; hence, the model described in [11] cannot be used for the description of the strain during the isothermal transformation.

The microstructural model developed in [12–16] was modified in [17] to describe the influence of long-term holding of the NiTi sample at room temperature on the two-way shape memory effect. This model includes the relationship between the martensitic transformation and the deformation defects (description of this type of defects is given in [17]), on one hand, and the relationship describing the evolution of these defects with time, on the other. This allowed an increase in the value of the two-way shape memory effect after long-time storage to be simulated. One may expect that this model can describe the strain variation during the isothermal martensitic transformation under stress. Against this background, the aim of the present work is to adjust the model developed in [12–17] to calculate the strain-time dependence obtained on holding of the NiTi-based alloy under different stresses at various temperatures near the M_s temperature.

2. Theory

According to the microstructural model given in [12–17], the representative volume of the alloy is considered as a number of grains, which may consist of the austenite phase and different martensite variants. The macroscopic small strain tensor is calculated as an average strain of all grains, and the strain of each grain is obtained as a sum:

$$\varepsilon^{(1)} = \varepsilon^{\mathrm{E}} + \varepsilon^{\mathrm{T}} + \varepsilon^{\mathrm{ph}} + \varepsilon^{\mathrm{MP}} + \varepsilon^{\mathrm{P}}, \qquad (1)$$

where ε^{E} is the elastic strain, ε^{T} is the thermal strain, $\varepsilon^{\mathrm{ph}}$ is the phase strain, $\varepsilon^{\mathrm{MP}}$ is the microplastic strain, and ε^{P} is the plastic strain. The elastic strain ε^{E} and thermal strain ε^{T} are calculated according to standard Hooke's law and the equation of thermal expansion, respectively. To find the phase εph and microplastic $\varepsilon^{\mathrm{MP}}$ strains, the following expressions are used:

$$\varepsilon^{\mathrm{ph}} = \frac{1}{N}\sum_{n=1}^{N}\Phi_n D^{(n)}, \qquad (2)$$

$$\varepsilon^{\mathrm{MP}} = \frac{1}{N}\sum_{n=1}^{N}k\varepsilon_n^{\mathrm{mp}}\,\mathrm{dev}D^{(n)}, \qquad (3)$$

where N is the number of martensite variants, Φ_n and $D^{(n)}$ are the volume fraction and the Bain's deformation of the n^{th} martensite variant, k is a material constant, and $\varepsilon_n^{\mathrm{mp}}$ is the measure of the microplastic strain originated by the growth of the n^{th} variant. The plastic strain is not considered in the present study, so the ε^{P} value is equal to 0. The conditions for the martensite transformations are given as:

$$F_n^{\mathrm{t}} = \pm F^{\mathrm{fr}}, \qquad (4)$$

where F_n^{t} is the generalized thermodynamic force causing the origination and growth of the n^{th} martensite variant, F^{fr} is a thermodynamic force resisting the transformation, sign "+" is for the direct transformation, and "–" is for the reverse transformation. These forces are calculated by the following equations:

$$F_n^{\mathrm{t}} = \left(\frac{q_0}{T_0}\left(T - T_0\right) + \sigma : D^{(n)}\right) - \mu\sum_m A_{mn}(f_m - b_m), \qquad (5)$$

$$F^{\mathrm{fr}} = -\frac{q_0\left(A_{\mathrm{f}} - M_{\mathrm{s}}\right)}{2T_0}, \quad \mu = -\frac{q_0\left(M_{\mathrm{s}} - M_{\mathrm{f}}\right)}{T_0}, \qquad (6)$$

where q_0 is the transformation enthalpy, T_0 is the temperature of the thermodynamic equilibrium, σ is the stress, A_{mn} is the matrix of different martensite variants interaction, b_m is the density of oriented defects associated with the m^{th} martensite variant (defects with oriented long-range stress field, produced by growth of m^{th} martensite variant), A_{f} is the finish temperature of the reverse transformation, and M_{s} and M_{f} are the start and finish temperatures of the forward transformation. A more detailed description of this model can be found in [17].

To take into account the possibility of isothermal transformation and related strain variation, the following explanation was used: during isothermal holding of the sample under a constant stress, the concentration of oriented defects can vary due to some relaxation process. The condition for the forward martensitic transformation (4) includes the force F_n^{t}, which depends on the density of the oriented defects b_n. Thus, the variation in bn value can lead to the fulfillment of the transformation condition (4) causing the martensite phase to grow at isothermal holding. The martensite transformation, in turn, can lead to a strain variation. To take this mechanism into account, a new equation was included in the model to describe the rate of microplastic strain measures $\varepsilon_n^{\mathrm{mp}}$:

$$\dot{\varepsilon}_n^{\mathrm{mp}} = r_{\mathrm{mp}}(T)\left(\frac{\left|F_n^{\mathrm{p}}\right| - F_n^{\mathrm{y}}}{\mu}\right)\mathrm{sign}\left(F_n^{\mathrm{p}}\right)H\left(\left|F_n^{\mathrm{p}}\right| - F_n^{\mathrm{y}}\right), \qquad (7)$$

where the dot indicates the time derivative of the corresponding variable, F_n^{p} and F_n^{y} are the generalized thermodynamic forces, the first of which causes the microplastic flow and the second describes the resistance associated with the non-oriented defects (scattered defects, which do not create oriented long-term stress field), and H is the Heaviside's function. The term $r_{mp}(T)$ corresponds to a relaxation process that controls the isothermal kinetics of the martensite transformation, and it is calculated according to formula:

$$r_{mp}(T) = r_{mp0} e^{-\frac{U_{mp}}{kT}}, \qquad (8)$$

where r_{mp0} is a model constant, k is the Boltzmann constant, U_{mp} is the activation energy, and M_s and M_f are the start and finish temperatures of the forward transformation. The equations for the defects concentration evolution have also been modified:

$$\dot{b}_n = k_b \dot{\varepsilon}_n^{mp} - k_b \frac{1}{\beta^*} |b_n| \dot{\varepsilon}_n^{mp} H\left(b_n \dot{\varepsilon}_n^{mp}\right), \qquad (9)$$

where b_n is the concentration of oriented defects, and k_b and β^* are model constants. According to these modifications, the system of Eqs. (4) – (9) allows the increments of ε_n^{mp} and Φ_n, which are used to calculate the phase and microplastic strains (detail description and formulas are given in [17]), to be determined. After that, the strain of representative volume can be found using formula (1).

3. Results and Discussion

The modified microstructural model was used to simulate the variation in the reversible strain of the $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy during isothermal holding under a stress of 235 MPa, which was previously experimentally studied in [8]. Transformation enthalpy and characteristic temperatures of the $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy in the stress-free state were previously measured by differential scanning calorimetry and published in [5 – 6], elasticity modules were determined during study of mechanical properties of the $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy. According to the Clausius-Clapeyron relation, the stress of 235 MPa increases the transformation temperatures to $M_s^\sigma = 325$ K, $M_f^\sigma = 298$ K, $A_s^\sigma = 337$ K, and $A_f^\sigma = 367$ K (these temperatures were measured using the $\varepsilon(T)$ curve obtained on cooling and heating under this stress). It is necessary to pay attention to the fact that the temperature range of the forward transformation under a stress was equal to 30 K, which was six times larger than without stress.

To determine the new parameters used in the modified model, such as r_{mp0}, U_{mp}, k_b, and β^*, the simulation of $\varepsilon(T)$ curves obtained on cooling and heating of the sample under a stress of 235 MPa was carried out and compared to the experimental curve. First of all, the parameters of the model were varied to make the experimental and simulated $\varepsilon(T)$ curves closer to each other (Fig. 1a). After that, the r_{mp0}, U_{mp}, k_b, and β^* parameters were varied to get the best correlation between the simulated and experimental $\varepsilon_{iso}(t)$ curves obtained for holding temperature equal to $M_s^\sigma - 6$ K (Fig. 1b). The best combination of r_{mp0}, U_{mp}, k_b, and β^* parameters are given in Table 1 as well as other material constants.

Fig. 2 shows the experimental and simulated curves obtained during cooling of the sample under a stress of 235 MPa to $M_s^\sigma - 6$ K, holding and heating under the same stress. On cooling, the strain increased due to the forward martensitic transformation, then strain additionally rose during isothermal holding under a stress. An increase in strain on holding was not due to the creep because this strain completely recovered on subsequent heating. It is seen that the simulated curve was close to the experimental one and allowed the strain variation on cooling, holding, and heating under a stress to be described.

Fig. 3 presents the experimental and simulated strain variation during isothermal holding of the alloy under 235 MPa at different temperatures (black lines are experimental results and red lines are simulated data). One may see that both experimental and simulated isothermal strain rose with time up to a saturation value depending on the position of the holding temperature relative to the M_s^σ temperature. A good agreement between the experimental and theoretical

Table 1. Material constants and modeling parameters used for simulation of isothermal martensite transformation.

Transformation temperatures [5 – 6]	$M_s = 284$ K, $M_f = 279$ K, $A_s = 302$ K, $A_f = 307$ K
Transformation enthalpy [5 – 6]	$q_0 = -150$ MJ/m^3
Elastic modulus of the austenite (E_A) and martensite (E_M) phases	$E_A = 76$ GPa $E_M = 25$ GPa
Poisson's ratio for the austenite (ν_A) and martensite (ν_M) phase	$\nu_A = 0.33$ $\nu_M = 0.45$
Activation energy U_{mp}	42 kJ/mol
Model parameters r_{mp0}, k_b, β^*	$r_{mp0} = 5000$ s^{-1} $k_b = 70$ $\beta^* = 5.5$

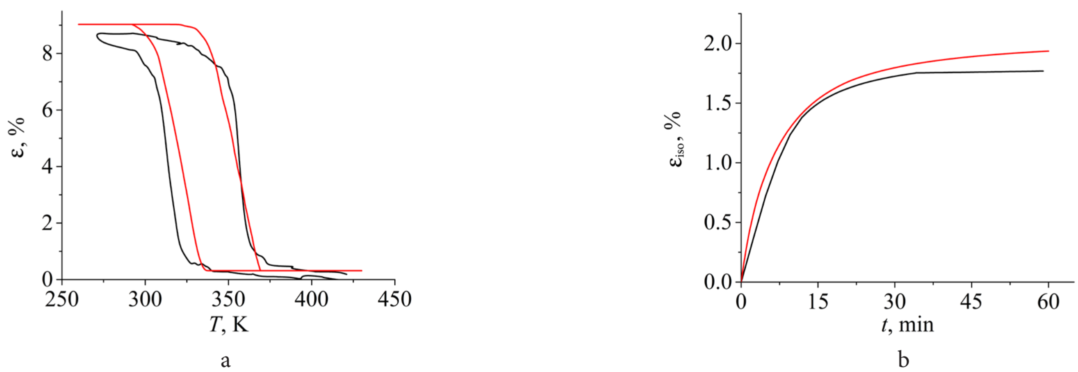

Fig. 1. (Color online) Experimental (black lines) and simulated (red lines) dependence of the strain on temperature obtained on cooling and heating of the $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy through the temperature range of the martensitic transformation under a stress of 235 MPa (a) and isothermal strain variation on holding of the alloy at the temperature of $M_s^\sigma - 6$ K under a stress of 235 MPa (b).

data was observed for holding temperatures $T^* < M_s^\sigma$ (Fig. 3b,c). At $T^* > M_s^\sigma$, the simulated curve was higher than the experimental curve, but the difference was not larger than 0.25% (Fig. 3a).

The strain, which appeared after 60 minutes of isothermal holding, was called the maximum isothermal strain, and Fig. 4a presents the simulated and experimental dependence of ε_{iso}^{max} on ΔT (difference between the holding temperature T^* and M_s^σ). One can see that both curves are non-monotonic, and the maximum value is observed at the same temperature equal to $M_s^\sigma - 6$ K. Calculation of $\varepsilon_{iso}^{max}(\Delta T)$ curves was carried out for the other values of the applied stress, and the results are presented in Fig. 4b. It was found that these dependences were also non-monotonic, with the maximum at $M_s^\sigma - 6$ K. An increase in stress caused a decrease in the maximum isothermal strain as it was found during the experimental study. So, it could be concluded that the modified microstructural model allows the holding temperature and stress at which the maximum isothermal strain can be found to be predicted.

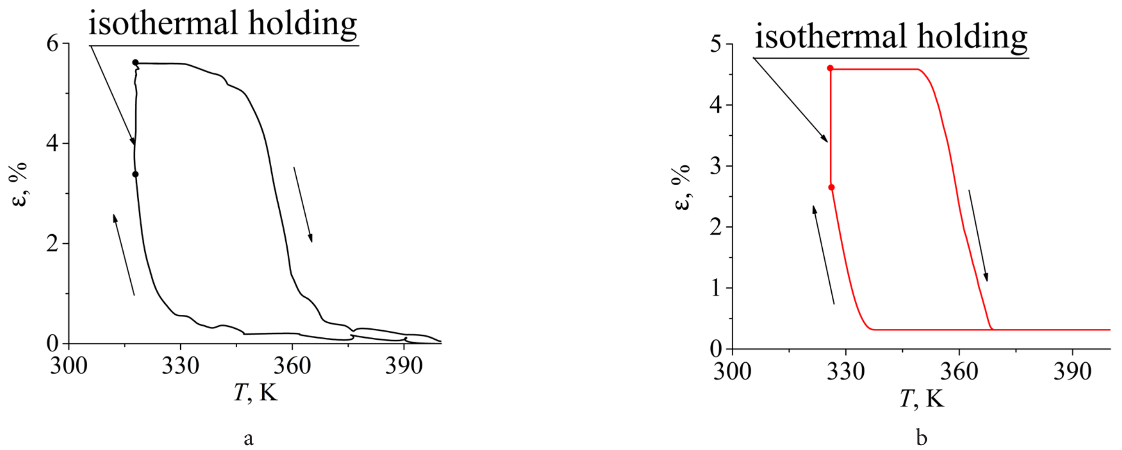

Fig. 2. (Color online) Variation in strain on cooling, isothermal holding at $M_s^\sigma - 6$ K and heating of the $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy: experimental (a) and simulated data (b).

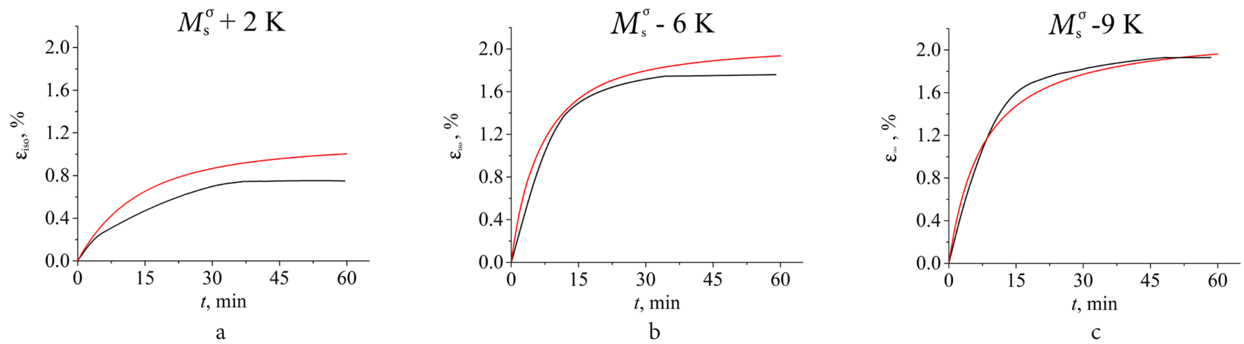

Fig. 3. (Color online) Simulated (red lines) and experimental (black lines) dependence of strain variation during holding of the alloy under a constant stress of 235 MPa at $M_s^\sigma + 2$ K (a), $M_s^\sigma - 6$ K (b) and $M_s^\sigma - 9$ K (c).

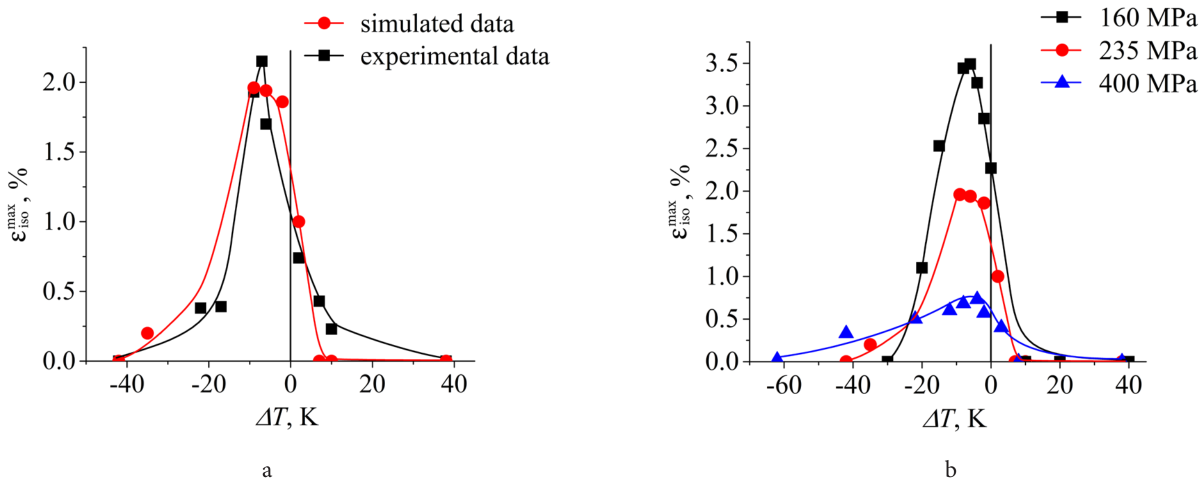

Fig. 4. (Color online) Simulated dependence of the maximum value of the isothermal strain on ΔT ($\Delta T = T^* - M_s^\sigma$, where T^* is the holding temperature): comparison with the experimental data obtained at 235 MPa (a) and with dependences calculated for different stress values (b).

4. Conclusions

The results of the study can be summarized as follows:

1. A description of the isothermal martensitic transformation on holding can be achieved by supplementing the "Likhachev-Volkov" microstructural model with equations accounting for a decrease in the concentration of oriented deformation defects due to the relaxation process.

2. The modified model allows the simulation of:

- recoverable strain variation on holding of the NiTi-based alloys under stress,
- non-monotonic dependence of the isothermal strain on the holding temperature, the temperature corresponding to the maximum isothermal recoverable strain being in agreement with the experiment,
- dependence of the isothermal strain on the stress that acted on holding.

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