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Simulation of recoverable strain variation during isothermal holding of the $Ni_{51}Ti_{49}$ alloy under various regimes

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The aim of the present paper is to simulate the strain variation on isothermal holding of Ni-rich NiTi alloy under various regimes. The modified Likhachev-Volkov microstructural model and a new Nelder-Mead algorithm for the determination of the model parameters were used. To determine the model parameters, the experimental data obtained during holding of the $Ni_{51}Ti_{49}$ alloy under a stress of 200 MPa were chosen. Using these parameters, the strain variation on holding of the NiTi alloy under a stress in two regimes was simulated. It was shown that the modified Likhachev-Volkov microstructural model allowed one to calculate the isothermal strain variation on holding after cooling under a stress (Regime 1) and a good correlation between the theoretical and experimental results were found. At the same time, the simulation of the strain variation on holding after active deformation (Regime 2) did not fit to experimental data because the model did not consider the difference in the stored elastic energy in two regimes. It was shown that a decrease in the elastic energy stored during the transformation increased the strain during holding under a stress after active deformation and made the simulated curves to be close to the experimental.

Keywords: microstructural model, isothermal holding, recoverable strain, shape memory alloys.

1. Introduction

The NiTi-based shape memory alloys are widely used in various applications due to their unique ability for a recovery of large unelastic strains on heating or unloading [1–3]. To simulate the behaviour of the shape memory alloys, different models are used [4–7]. Nowadays, the strain and stress variation may be simulated on temperature and stress variation under various regimes. However, all these models are based on the athermal kinetics of the martensitic transformation. At the same time, previously, it was shown that the recoverable strain variation might be observed not only on temperature or stress variation but it took place on isothermal holding of the samples at a constant temperature and stress [8–10]. This was caused by the thermal elastic martensitic transformation in non-stoichiometric NiTi alloys which might occur under isothermal holding due to a variation in the local concentration of substitutional atoms (the detailed description of the mechanism for the observation of the martensitic transformation during isothermal holding was given in [11]). It was shown that if holding was carried out under a stress, then the martensitic transformation was accompanied by the strain variation [8–10]. On subsequent heating or unloading the strain accumulated on holding recovered during the reverse transformation. Thus, the isothermal holding under a stress might be used as a new way for the pre-deformation of NiTi-based alloys.

One may assume that it is not possible to use the model describing the athermal martensitic transformation to simulate the strain variation on holding under a stress. However, in [12] it was shown that the modification of the Likhachev-Volkov microstructural model described in [12–14] allowed one to simulate the strain variation on holding of the NiTi-based alloys. To take into account the isothermal variation in the martensite volume fraction on holding, it was suggested that 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. This assumption allowed simulating the strain variation of the $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy on cooling — holding — heating under a stress of 235 MPa. The influence of the holding temperature and stress on the isothermal strain was described and a good correlation between the theoretical and experimental data was found [12].

Therefore, the modified Likhachev-Volkov microstructural model can be used for the simulation of the isothermal strain variation on holding of the NiTi-based shape memory alloys under a stress. However, this model had a complex procedure for the determination of the model parameters. To carry out this procedure, a lot of experimental data should be obtained and used for the calculation that made the using of this model difficult. In [15], a new algorithm was proposed for the determination of the parameters for the modified Likhachev-Volkov microstructural model which was based on solving of the problem for minimization of some non-negative fitness function corresponding to the difference between experimental and simulated data. This function can be written as follows:

$$\text{fitness(parameters)}=\sum_{i=1}^{N} w_i\left(\chi_i^{\text{theory}}-\chi_i^{\text{exp}}\right)^2, \qquad (1)$$

where w_i the weight coefficients, χ_i^{theory}, χ_i^{exp}, simulated and experimental parameters which are used for the minimization of the “fitness” function. The weight coefficients w_i are chosen to make the terms of the fitness function to be of the same order. The closer the value of this function to zero, the less the difference between the simulated and experimental data. To minimize the fitness function, the Nelder-Mead method can be used [16]. Such an algorithm was used in [15] to determine the parameters for the modified Likhachev-Volkov microstructural model. It was shown that this algorithm simplified the procedure for the determination of the parameters because it was not necessary to use a lot of experimental curves. The aim of this work was to use a new algorithm for the determination of the model parameters and the modified Likhachev-Volkov microstructural model to simulate the strain variation on holding of the $Ni_{51}Ti_{49}$ alloy under various regimes.

2. Computational procedure

To determine the model parameters, the algorithm described in [15] was used. At the first step, the "fitness" function included four parameters (χ_i): the start and finish temperatures of the martensitic transformation, strain recovered on heating and irrecoverable strain which were determined on cooling and heating under a stress of 200 MPa. The minimization of this function allowed one to obtain the simulated strain vs temperature curve that correlated to the experimental curve and determine the set of model parameters which were used as the initial parameters for the second step of the minimization. At this step, the fitness function included 6 parameters: the start temperature of forward transformation under a stress, the strain of the alloy before holding, strain recovered on heating after holding, irrecoverable strain, the strain increased on holding for 60 min, and the strain rate at the beginning of holding which were determined on cooling — holding — heating under a stress of 200 MPa. The minimization of the fitness function at this step allowed obtaining a final set of the model parameters which are given in the Table 1 (the detailed description of the model parameter determination procedure is given in [15]). Besides these parameters which were variable, the elastic modulus of the austenite or martensite phases, Poisson's ratio, yield limit for dislocation slip and yield limit for the detwinning were used as constants and were not changed.

Figure 1 shows the strain vs time curves obtained on holding under 200 MPa at different temperatures (Fig. 1a) and the influence of the holding temperatures on the isothermal strain (strain increases on holding under a stress) (Fig. 1b) which were simulated using a final set of the model parameters shown in Table 1. A good correlation between the simulated and experimental data confirms that the chosen algorithm for the determination of the parameters for the modified Likhachev-Volkov microstructural model can be successfully used for the simulation of the strain variation on isothermal holding under a stress.

3. Results and discussion

The set of parameters shown in Table 1 was used to simulate the strain variation on holding of the $Ni_{51}Ti_{49}$ alloy under two regimes which were used in the experimental study [10]. In Regime 1, the sample was subjected to cooling, holding and heating under a stress of 100 or 300 MPa. In Regime 2, the sample was cooled to the holding temperature without stress, loaded to a stress of 300 MPa, held under the stress and unloaded. Figure 2 a shows the simulated strain vs temperature curve obtained in Regime 1 when the holding was carried out under 300 MPa. It is seen that the strain increases both on cooling under 300 MPa and on holding. On heating the strain completely recovers. In the second regime, the strain increases on tension to 300 MPa and on further holding (Fig. 2b). On unloading, the strain completely recovers.

Table 1. The values of the parameters for the modified Likhachev-Volkov microstructural model which were determined using a Nelder-Mead minimization of "fitness" function and the model constants.

Parameter*	Description	Value
M_f*	Characteristic temperatures of martensite transformation	−63°C
M_s*		−45°C
A_s*		−28°C
A_f*		−11°C
q_0*	Latent heat of transformation	−72 MJ/m^3
α*	Coefficient responsible for the interaction of martensite variants	0.0
r_{mp0}*	Multiplier (r) and activation energy (U) for the Arrhenius dependence in the equation for microplastic strain variation	$1.86\cdot10^4$ s^{-1}
U_{mp}*		39 кJ/mol
m_{mp}*	Model Parameter	3.5
a_y*	Coefficient of isotropic hardening	$2.1\cdot10^5$ MPa
β*	Model Parameter	5.2
k_b*	Relation coefficient of micro plastic strain and oriented defects	81
k_{mp}*	Microplastic strain scaling factor	2.3
E_A**	Young Modulus of austenite phase	70 GPa
E_M**	Young Modulus of martensite phase	40 GPa
ν**	Poisson's ratio	0.33
τ_{yield}**	Yield limit	185 MPa
σ_{tw}**	Twinning limit	20 MPa

* The variable parameters which were determined in this paper (expressions for their determination are given in [15]).

** The constants which were not varied in this paper.

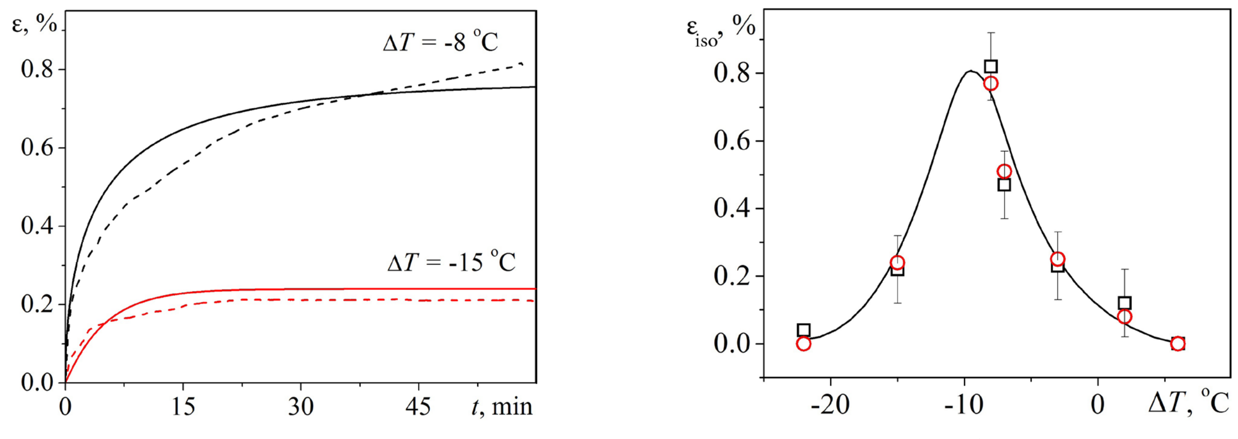


Fig. 1. (Color online) Simulated (solid line) and experimental (dashed line) strain vs time curves obtained on holding of the $Ni_{51}Ti_{49}$ alloy under a stress of 200 MPa (a). The influence of the difference between the holding temperature and the start temperature (M_s) of the forward transformation on isothermal strain observed after holding under a stress of 200 MPa (b). In Fig. 1b, black squares are the experimental results, red circles are the simulated data.

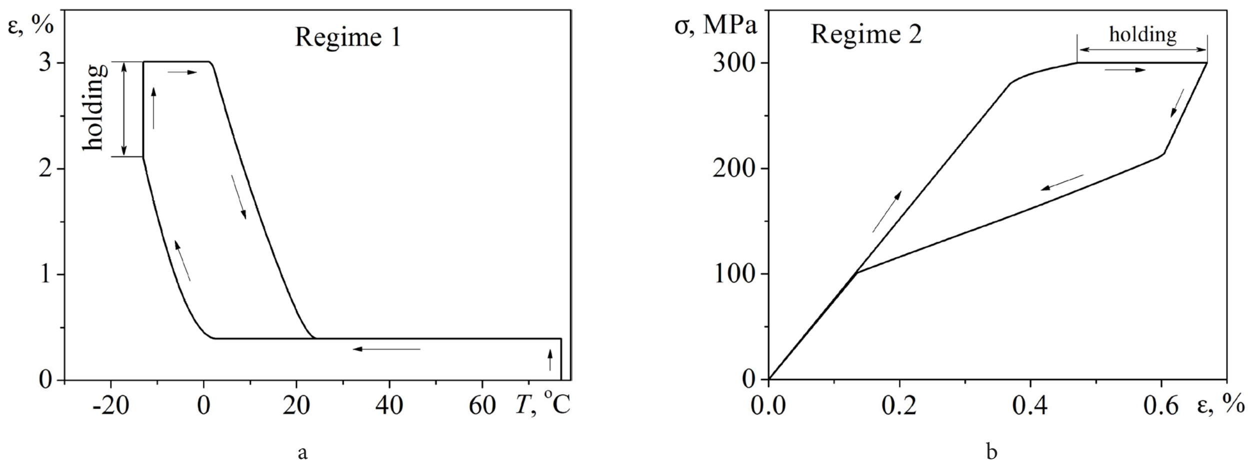


Fig. 2. The strain vs temperature curve obtained on simulation of strain variation on cooling — holding — heating under a stress 300 MPa (a). The simulated stress vs strain curves obtained on tension — holding — unloading at constant temperature (b).

The simulated results were compared to the experimental data taken from [10]. Figure 3 shows the experimental and simulated strain vs time curves obtained on holding in Regime 1 under a stress of 100 or 300 MPa. In Fig. 3a, one can see that if the stress acting on holding was 100 MPa, then the difference between the experimental and simulated data was within 0.1% that was close to the error for the strain measurement by a video-extensometer (see the details of experimental results in [10]). If the stress on holding was 300 MPa, then the difference between the experimental and simulated data depended on the holding temperature (Fig. 3c), that may be caused by the experimental error in the determination of the ΔT value (the difference between the holding temperature and the M_s temperature). The error for the temperature measurement was 1°C, hence the error for the ΔT value might be equal to 2°C. At the same time, the variation in holding temperature led to a significant change in the isothermal strain (Fig. 3b, d).

Using the $\varepsilon(t)$ curves obtained experimentally and by simulation, the strain variation on holding for 60 min (ε_{iso}) was found and the influence of the holding temperature on the isothermal strain was analysed (Fig. 4). It is seen that a variation in the ΔT value led to a non-monotonic variation in the isothermal strain and the experimental and simulated data were close to each other. Thus, the results of this paper correlate to the data published in [10] and hence the modified Likhachev-Volkov microstructural model where the parameters have been determined using a new algorithm allows one to simulate the strain variation on holding of the $Ni_{51}Ti_{49}$ alloys in Regime 1 under various stresses.

In Regime 2, the holding was carried out after active tension to holding stress (Fig. 2b). Figure 5 shows the simulated and experimental stress vs strain curves found on holding under this regime (loading to 300 MPa, holding and unloading). It is seen that a huge difference was found between the simulated and experimental data. The isothermal strain variation was 6% on holding in experiments and only 0.2% on simulation.

The large discrepancy between the simulated and experimental data was found for all holding temperatures and holding stress in Regime 2. This may be caused by the fact that the modified Likhachev-Volkov microstructural model does not take into account the differences in the variations of the stored elastic energy during the transformation in Regimes 1 and 2. In [10] it was experimentally shown that the isothermal transformation was accompanied by a large stored elastic energy in Regime 1. This led to a partial suppression

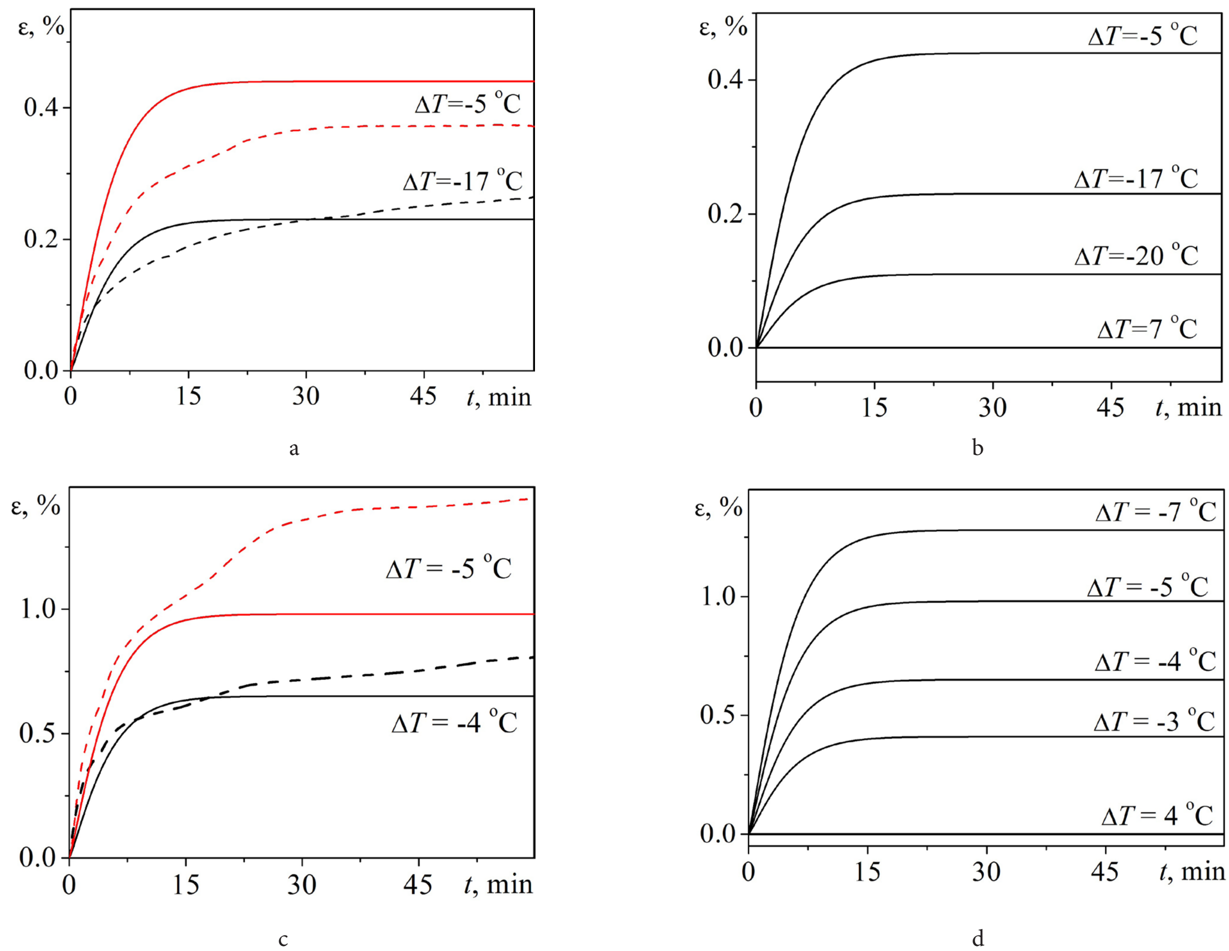


Fig. 3. (Color online) Strain variation on holding of the $Ni_{51}Ti_{49}$ alloy under a stress of 100 MPa (a, b) or 300 MPa (c, d). Experimental results — dashed lines; simulated data — solid lines. ΔT is the difference between the holding temperature and the M_s temperature.

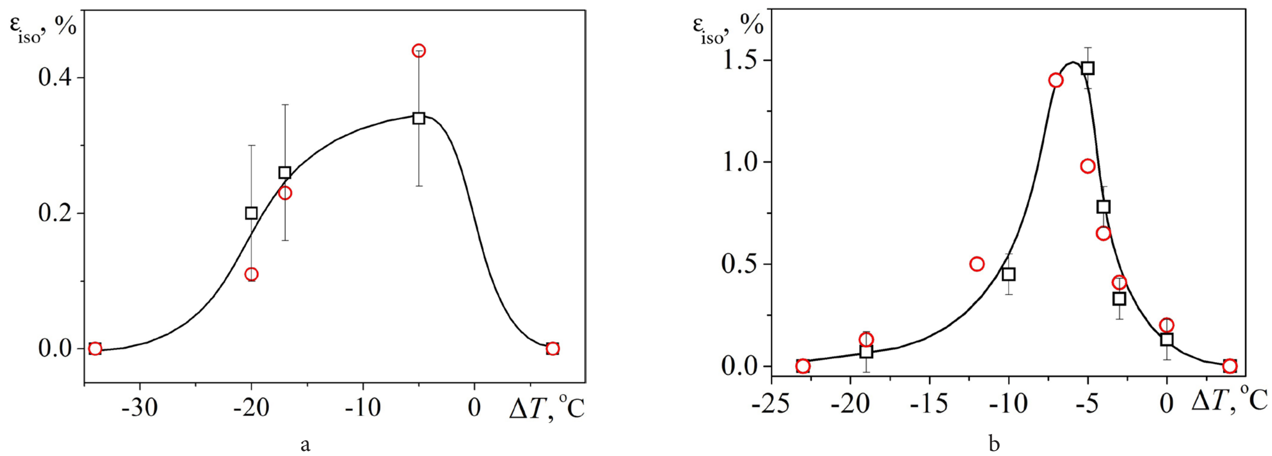


Fig. 4. (Color online) Dependencies of the isothermal strain on the difference in the holding temperature and the M_s temperature obtained when holding was carried out under 100 (a) or 300 MPa (b). Black square symbols are experimental results; red circle symbols — simulated data.

of the variation in the volume fraction of the martensite on holding and, as a result, the isothermal strain was small. At the same time, the isothermal transformation in Regime 2 was accompanied by a small stored elastic energy, and a large isothermal strain was found. The reason for the difference in the variation of the stored elastic energy in two regimes have not been clarified yet, that is why it cannot be considered in the modified Likhachev-Volkov microstructural model. However, the stored elastic energy in the model may be artificially changed by the variation in the temperature range of the forward transformation (the difference between the start (M_s) and finish (M_f) temperatures of the forward transformation). To check whether the isothermal strain observed on holding in Regime 2 depended on the stored elastic energy, the strain variation was simulated in Regime 2 with different M_s-M_f values (other model parameters were not changed). Figure 6 shows the stress vs strain curves simulated for different M_s-M_f values. It is seen that a decrease in the M_s-M_f value increases the isothermal strain that confirms the assumption given in [10].

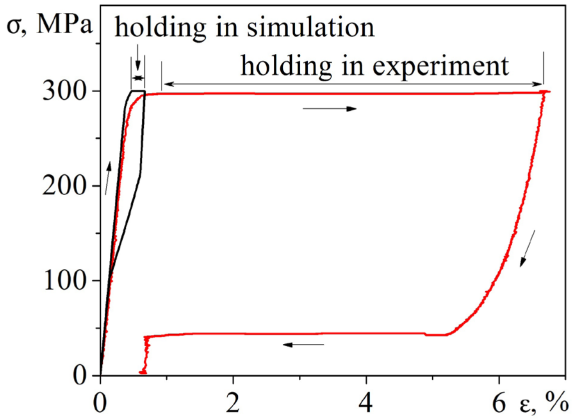


Fig. 5. (Color online) Experimental (red) and simulated (black) stress vs strain curves obtained on tension of the $Ni_{51}Ti_{49}$ alloy to 300 MPa, holding for 60 minutes and unloading. Before active deformation, the sample was cooled to holding temperature without stress. Holding temperature was equal to a temperature at which the forward transformation started on cooling under a stress of 300 MPa.

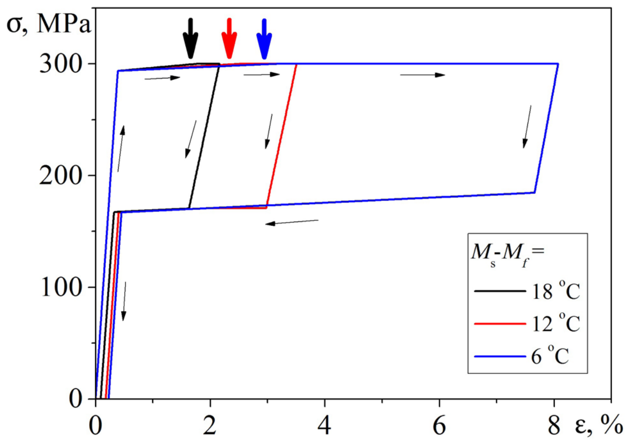


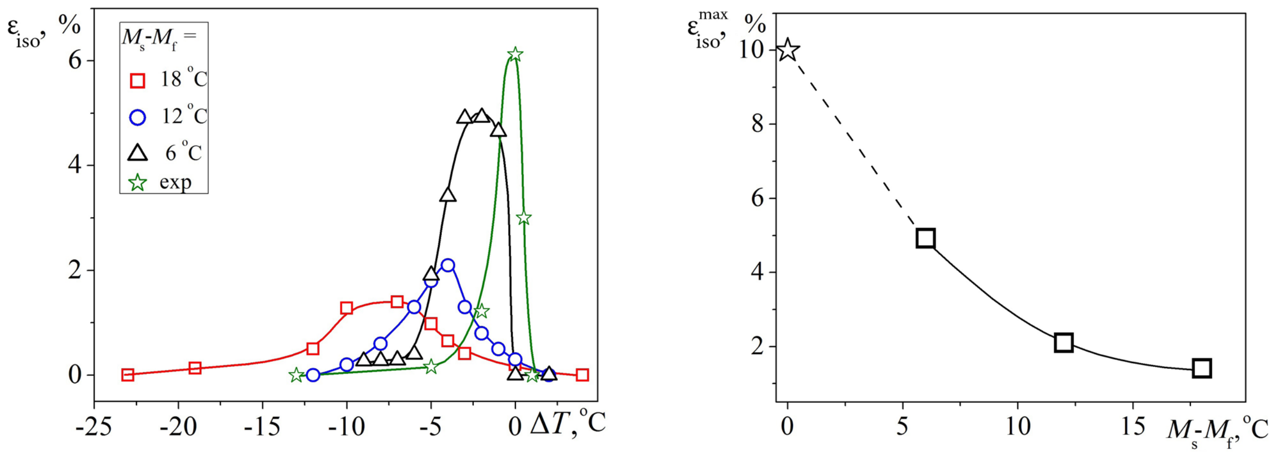
Fig. 6. (Color online) Simulated stress vs strain curves obtained on holding of the $Ni_{51}Ti_{49}$ alloy under a stress of 300 MPa at different M_s-M_f values. $\Delta T = -3$°C. Colored arrows show the start of holding.

The stress vs strain curves were simulated for holding of the $Ni_{51}Ti_{49}$ alloy at various holding temperatures and various M_s-M_f values and Fig. 7a shows the ε_{iso} (ΔT) dependences. It is seen that a decrease in the M_s-M_f value leads to an increase in the isothermal strain and decreases the temperature range where holding under 300 MPa is accompanied by the strain variation. If M_s-M_f=18°C, as it was used in simulation shown in Fig. 5, then the maximum isothermal strain was equal to 1.4% and the isothermal strain was observed in the temperature range 0°C < ΔT < 20°C. If the M_s-M_f was decreased in tree times and equal to 6°C, then the maximum isothermal strain increased by 5% and the isothermal strain variation was found in the temperature range 0°C < ΔT < 6°C. Moreover, it is seen that at M_s-M_f = 6°C, the simulated curve became close to the experimental curve. This confirms the conclusions that a variation in stored elastic energy affects the isothermal strain. Figure 7b shows the influence of the M_s-M_f value on the maximum isothermal strain. It is seen that if M_s-M_f decreases to zero, then the maximum isothermal strain increases by 10% that was close to the crystallography resource of the transformation in NiTi-based alloys. Using this simulated ε_{iso}^{max}(M_s-M_f) curve and the experimental value of the maximum isothermal strain, one can determine the M_s-M_f value which should be taken in the model to simulate the isothermal strain variation on holding in Regime 2.

4. Conclusions

The results of the study can be summarized as follows:

1. Modified Likhachev-Volkov microstructural model for the behavior of shape memory alloys with a new algorithm for the determination of the model parameters can be successfully used for the simulation of the strain variation during the isothermal holding in Regime 1.
2. The variation in the M_s-M_f value affects the isothermal strain on holding. A decrease in the M_s-M_f values increases the isothermal strain and decreases the temperature range where the isothermal holding under a stress is accompanied by the strain variation.
3. To describe the strain variation on holding in Regime 2, the M_s-M_f value should be estimated using the



a b

Fig. 7. (Color online) The influence of the M_s-M_f value on the dependence of the isothermal strain on the holding temperature (a) and on the maximum isothermal strain (b) observed on holding under 300 MPa. Black, red and blue are the simulated data; green is the experimental result.

$\varepsilon_{iso}^{max}(M_s\text{-}M_f)$ curve found in the present study and the maximum isothermal strain measured on experimental holding. The value obtained should be used in modified Likhachev-Volkov microstructural model to simulate the strain variation on holding under a stress after active loading.

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