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A Model of Martensitic Unelasticity Accounting for the Crystal Symmetry of the Material

I.V. Erglis, V.A. Ermolayev and A.E. Volkov

Res. Inst. Math. Mech. (NIIMM) St.-Petersburg State Univ., Bibliotechnaya pl. 2, Petrodvorets, 198904 St.-Petersburg, Russia

Abstract. An approach is presented to describe the mechanical behavior of the shape memory materials. On the one hand it uses the basic concepts of the structure-analytical theory proposed by V.A.Likhachev and V.G.Malinin which are the formulation of the constitutive equations of the phase transformation and martensitic unelasticity for micro regions and the orientation averaging of micro strains to obtain the macro strain. On the other hand the averaging procedure is arranged in a way to account for the crystal symmetry of the material. Results are presented of the computer simulation of pseudoelasticity, shape memory effect and active straining of a shape memory material with a thermoelastic martensitic transformation. These are stress-strain diagrams at various temperatures, temperature dependencies of the martensitic unelastic strain. All the results show good qualitative agreement with the experiments in which dislocation plasticity does not play a significant role.

1. INTRODUCTION.

In recent time many approaches have appeared which can describe the mechanical behaviour of alloys with martensitic transformations. These works account for various features of martensitic transformation. In [1-3] the description of materials with martensitic transformations is built based mainly on the thermodynamical aspects of transformations. An entirely mechanical approach has been developed in [4]. Large success has been achieved in describing the strain of an alloy due to pseudoelasticity, transformation plasticity and strain recovery. One of the most successful was the structure-analytical theory of plasticity and strength [5,6] which tries to combine physical and mechanical approaches to this problem. The deformation is considered as a process developing on two levels: macroscopic - in which ensembles of grains are considered as points of the medium - and microscopic in which separate martensite single crystals are distinguished. The observed macroscopic strain is then the mean value of micro strains. Kinetics of the microstrain is described by some differential equations accounting for the basic phenomenological data on the transformation kinetics. The difficulties of the space averaging procedure are overcome by its replacing to the orientation averaging as in the theory of slip. This approach has managed to model qualitatively the deformation of an alloy with martensitic transformations of the first order under simultaneous action of varying stress and temperature. The present work makes an attempt to bring the structure-

analytical theory closer to crystallographical aspects of the transformation and thus to obtain better agreement with experimental data. It differs by the averaging procedure which is organized in a way to account for the possibility of realizing in the same grain of several crystallographically equivalent variants of the transformation. This has allowed to obtain better quantitative agreement with experimental data on titanium nickel mechanical behaviour.

2. FORMULATION OF THE MODEL

We base on the following very simple assumptions about the martensitically unelastic material. We consider that it consists of grains numbered $1, 2, \dots, \omega, \dots, \Omega$ each being a single crystal. In a grain martensite can appear in N crystallographically equivalent variants characterised by transformation strains

$$D_n = P_n D P_n^{-1}, \quad n = 1, 2, \dots, N \quad (1)$$

where D is the transformation strain matrix for one of the variants referred to the crystal physical basis of austenite; P_n , $n=1, 2, \dots, N$ are rotation matrixes belonging to austenite crystal symmetry group and D_n is the strain matrix for the n -th variant. We imply that transformation strain is the pure (Bain's) strain of the transformation. The amount of martensite obtained through the n -th variant we will characterize by the quantity Φ_n such that $(1/N)\Phi_n$ is the volume fracture of this martensite. If the transformation occurred in an unstressed grain then all martensite variants would occupy equal volumes and their volume fracture would be $1/N$. Thus Φ_n is the ratio of the volume of the n -th martensite variant to the volume it would occupy if the transformation had occurred in an unstressed grain.

The mean strain matrix ε^{gr} of a grain due to the transformation in these notations is

$$\varepsilon^{gr} = \frac{1}{N} \sum_{n=1}^N \Phi_n D_n \quad (2)$$

Passing to the laboratory basis and averaging the strain of all the grains we will calculate the macroscopic martensitically unelastic (martensitic) strain matrix ε^m of the material:

$$\varepsilon^m = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} R_{\omega} \varepsilon_{\omega}^{gr} R_{\omega}^{-1}, \quad (3)$$

where $\varepsilon_{\omega}^{gr}$ is the mean strain matrix in the grain number ω and R_{ω} is the rotation matrix turning the laboratory basis into the crystal physical basis of grain ω .

The evolution law for Φ_n in any of the grains was the same as in the structure-analytical theory [5.6]:

$$\begin{aligned} \Phi_n = & -\frac{\dot{T}^*}{M_s - M_f} H(-\dot{T}^*) H(1 - \Phi^{gr}) H(M_s - (M_s - M_f)\Phi_n - T^*) - \\ & -\frac{\dot{T}^*}{A_f - A_s} H(\dot{T}^*) H(\Phi_n) H(T^* + (A_f - A_s)\Phi_n - A_f) \end{aligned} \quad (4)$$

where M_s , M_f , A_s , A_f are the characteristic temperatures of the martensitic transformation, H is the Heaviside's function, $\Phi^{gr} = \frac{1}{N} \sum_{n=1}^N \Phi_n$ is the volume fraction of martensite in this grain and T_n^* is the effective temperature for the n -th martensite variant. It is introduced into theory to account for the stress effect on the transformation. In conformity with the Clausius - Clapeyron equation it is determined by the formula

$$T_n^* = T + \frac{\tau \cdot D_n}{q_0} \quad (5)$$

where T is the absolute temperature, T_0 is the phase equilibrium temperature, q_0 is the enthalpy of the transformation (negative for the direct transformation in TiNi) and τ is the stress matrix in the crystal physical basis of the grain.

The elastic strain of the material was calculated by isotropic Hook's law independently for martensite ($\epsilon^{el,M}$) and austenite ($\epsilon^{el,A}$) and the mean elastic strain ϵ^{el} was calculated with the use of the mixture rule:

$$\epsilon^{el} = (1 - \Phi_M) \epsilon^{el,A} + \Phi_M \epsilon^{el,M} \quad (6)$$

where $\Phi_M = (1/\Omega) \sum \Phi_n^{gr}$ is the volume fraction of martensite, the sum taken on all the grains.

3. RESULTS OF MODELLING.

The described above model has been applied to simulate the main phenomena of martensitic unelasticity, namely active axial loading at various temperatures, transformation plasticity when cooling the stressed material, strain recovery in the course of the reverse transformation. The model material consisted of 100 grains orientations of which were uniformly distributed in the orientation space. The austenite grain lattice was assumed to be cubic with 24 elements of symmetry. The deviator part of the transformation strain D

describing the B2 - B19' transformation in TiNi was taken from [7] and its isotropic part was chosen to give the transformation dilatation equal - 0.34% as it is in TiNi. Other transformation characteristics were: $M_s = 300$ K, $M_f = 280$ K, $A_s = 340$ K, $A_f = 360$ K, $T_0 = 330$ K, $q_0 = -200$ MJ/m³. Young's moduli were 68 GPa for martensite and 74 GPa for austenite, Poisson's ratios equaled 0.48 and 0.33 respectively. No adjusting constants were used. Heat expansion and dislocation plasticity were not taken into account so the results where stress exceeds dislocation flow limit of course can not be compared with the real experiment.

Stress - strain diagrams (fig.1) show good qualitative agreement with the experiment and the same order of strain values. At $T > A_f$ there is full pseudoelastic strain recovery and the residual strain is present after unloading at $T < A_f$.

The transformation plasticity in cooling and the strain recovery in consequent heating is shown in fig.2 and fig.3. When the material is "cooled" without stress it accumulates a small negative strain due to the dilatation effect of the transformation. We have tested that if the transformation strain tensor is replaced by its deviator no strain is produced in cooling. When the transformation plasticity strain was produced at small stresses one can see kinetics of the strain recovery normally observed in experiments, that is the recovery temperatures are higher than those of the strain accumulation in preceding cooling under a constant stress. (fig.3a). But when the same model experiment was held for greater stresses (curve for 600 MPa in fig.3b), character of the accumulation - recovery kinetics changed and the recovery branch of the graph lay to the left of the accumulation one. This happened when the stress was nearer to the values delivering saturation to the maximum transformation plasticity strain as function of the stress. This dependence is plotted in fig4 and it is linear for small values of the stress (not exceeding 250 MPa). In fig3 one can also notice a considerable shift with the stress of the strain production start and strain recovery finish temperatures and a very weak stress dependence of the strain production finish and strain recovery start temperatures.

Fig.5 shows quite ordinary strain recovery after residual strain had been produced in the material by tension at 280 K (that is at M_f). Shift of the strain recovery start temperature with the growth of residual strain can be observed. Fig.6 illustrates heating under a constant stress. On the first stage the strain is accumulated in the direction of the stress and on the second stage it recovers. The explanation of this phenomenon is, that martensite obtained by cooling of the unstressed material consists of crystallites belonging to all the variants of the transformation. When it is heated under a stress first turn into austenite the crystallites the reverse transformation strain of which delivers maximum work to the applied stress. On the final stages of the transformation all the martensite crystallites disappear with the full strain recovery.

4. CONCLUSION and ACKNOWLEDGEMENTS

The results of computer modelling presented above show that the proposed approach possesses all positive features of the structure-analytical theory. It correctly describes all main aspects of shape memory materials mechanical behavior such as the active

Figure 1. Calculated stress-strain diagrams at various temperatures (figures at curves in K).

Figure 2. Strain versus temperature in cooling and heating under various constant stresses (figures at curves in MPa)

Figure 3. Strain versus temperature for transformation plasticity in cooling under various constant stresses (figures at curves in MPa) and strain recovery in heating of the unstressed material. a - small stresses, b - larger stresses.

Figure 4. Dependence of the maximum transformation plasticity strain on the stress in cooling.

Figure 5. Strain recovery after active axial loading by various stresses (figures at curves in MPa) of martensite at 280 K.

Figure 6. Strain dependence on temperature for model material loaded by various stresses (figures at curves in MPa) at 250 K and heated.

deformation at various temperatures, transformation plasticity and shape memory effect. At the same time it demonstrates better quantitative agreement with experiments concerning the transformation plasticity strain and the shift of temperatures at which strain variation start and finish is observed.

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