Simulation of Shape Memory Devices with Coupled Finite Element Programs

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ABSTRACT

This paper presents thermal and mechanical calculations on micro devices driven by electrical heating of a shape memory alloy (SMA). For simulation a program package has been developed to allow coupling of single task Finite Element Method (FEM) -programs in an arbitrary sequence, which enables the calculation and optimization of the performance of complex micro systems [1]. Electrical and thermal calculations are performed with the FEM program Tosca[2], which was extended by the authors to become a time dependent program for thermal analysis. For the mechanical calculation a three dimensional FEM program has been developed, which is based on a two phase model including history effects to describe the shape memory material.

1 INTRODUCTION

SNA microactuators are heated by electrical currents gain growing interest for use in micro systems. Microvalves for fluidic applications, micro grippers for positioning and manufacturing and micro optical switches have already been developed [3]. The advantage of shape memory actuators ar large forces even in low dimensions. No problem arises due to electrical charge like in electrostatic devices. Designing such actuators, the principal task is to determine temperatures, displacements and stresses as function of the heating current. For complicated structures three different FEM calculations must be done. First, the electrical current distribution in the actuator is calculated, which determines the electrical heating power. This allows the calculation of the thermal distribution. Then the thermal results are passed to a mechanical solver which must be able to calculate stresses and displacements for SMA materials. For optimization a lot of these coupled simulations are needed and it is desirable to run it automatically. For this purpose we apply a FEM coupling scheme as presented in [1]: An overlying program ("Regie-program") starts all involved FEM programs and programs for data transfer. First, we will discuss some details of the calculation procedure. Then we apply this package for calculation of displacements of a thin SMA cantilever beam including history effects and for calculation of the temperature and stress distributions in SMA microvalves.

2 SIMULATION PRECEDURE

During the coupled simulation the following physical properties are calculated:

2.1 Electrical Calculation

The electrical current density j is determined by the program Tosca [2]. At the electrical connections a Neuman boundary condition exists:

$$\sigma\bar{\nabla}U = j_0 . \qquad (1)$$

The parameter σ denotes the electrical conductivity, U is the electrical potential. At surfaces of symmetry, a Dirichlet boundary is given (e.g. U = 0). From j the heating power q is calculated by integrating the product $\sigma(\nabla U)^2$ over the finite element volume by the program Script_tosca which also changes the material and boundary values in the Tosca data base to the corresponding thermal problem.

2.2 Temperature Calculation

Assuming isotropic materials, the heat-transfer problem within a three-dimensional device is defined by the differential equation

$$m(c_p + h(T))\dot{T} = q - \lambda\Delta T , \qquad (2)$$

which takes into account the sensible heat, the heat of phase transformation *h(T)*, the heating power generated by electrical current q and losses due to heat conduction. The parameters m, c_p and λ denote the mass, specific heat capacity and thermal conductivity, respectively. At the device surface, the following boundary condition is considered:

$$-\lambda\bar{\nabla}T = K(T - T_E) , \qquad (3)$$

which takes into account the convective heat exchange with the environment of temperature T_E. The parameter K denotes the heat-transfer coefficient. At surfaces of symmetry the Neuman boundary $\nabla T = 0$ is given. For these calculations the program Tosca was extended with a mass matrix and additional source terms to describe The phase transformation. For the time dependent analysis we use a Crank Nicolson scheme.

2.3 Mechanical Calculation

Three dimensional mechanical simulations are done with the FEM code Brick28, which offers two options for the SMA simulation: - The use of temperature dependent stress-strain characteristics determined by experiments on test devices or the use of a simplified two phase model as given e.g. by Ikuta [4]. The latter has been extended to three dimensions for the calculations done in this paper. In the model, the Martensitic (M) phase and Austenitic (A) phase are parallelly connected in each volume fraction . Thus, the total stress $\{\sigma\}$ as function of strain $\{\varepsilon\}$ is given by:

$$\{\sigma\} = R_A \{\sigma_A(\varepsilon)\} + R_M \{\sigma_M(\varepsilon, \varepsilon_p)\} \quad (4)$$

R_A and R_M are the mean volume fraction of A-phase and M-phase, respectively. They are given by:

$$R_M = 1/(1+\exp[k(T-T_0 - c\,\sigma^*)])\,; \quad R_A = 1 - R_M \quad (5)$$

For heating processes T_0 and k depend on the start and end temperature of the austenitic phase A_S and,A_F and for cooling processes on the start and end temperature of the martensitic phase M_S and M_F. . These values may be determined experimentally. For σ^* the effective stress is used. The parameter c is determined to 1/6 K/Mpa. The mechanical property of the A-phase are calculated by completely linear elastic analysis:

$$\{\sigma_A(\varepsilon)\} = E_A \mathbf{D_0} * \{\varepsilon\} \quad (6)$$

$\mathbf{D_0}$ is the conventional matrix of elastic constants of isotropic media, E_A is the elastic modulus of the A-phase.
A nonlinear stress–strain relation, shown in Fig. 1. is considered for the M-phase:

$$\{d\sigma_M(\varepsilon)\} = E_M \mathbf{D_0} * (\{d\varepsilon\} - \{d\varepsilon_p\}) = E_M \mathbf{D_p} * \{d\varepsilon\} \quad (7)$$

$\mathbf{D_p}$ is the plastic matrix e.g. given by [5], $d\varepsilon_p$ is the increment of plastic deformation caused by twin deformation.

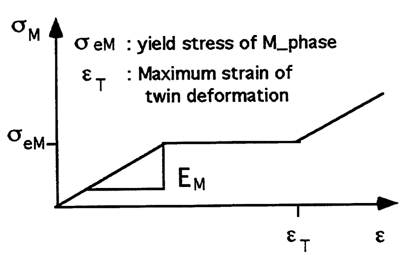

Figure 1: Stress-Strain model for the M-phase.

The elemental tangent stiffness matrix K_T is given by:

$$K_T = \int B^T * (R_A E_A \mathbf{D_0} + R_M E_M \mathbf{D_p}) B \; dv \quad (8)$$

Where matrix B relates strain $\{\varepsilon\}$ and displacements $\{a\}$. For B we use the form given by Zienkiewicz [6], in which B is split of in a small displacement part B_0 and a part $B_l(a)$ linear dependent on the displacements: $B = B_0 + B_l(a)$.

In a first solution step we estimate R_M for zero stress. Then ,neglecting plastic deformation we solve the nonlinear displacement problem with a Newton Raphson method described in [6]. After convergence the displacements and stresses are used as first approximation for a modified incremental tangent stiffness method given by R. D. Cook [5] to solve the nonlinear problem:

$$\Sigma K_T a = f + f - \Sigma \int B^T * \sigma \, dv \quad (9)$$

f are the applied external loads and the sum extends over all elements.. At each iteration step a new value of R_M and R_A is calculated from the actual stress data.

2.4 History effects

In the case of partial phase transformation, when the SMA material is cooled down to a temparature $T_1 > M_F$ and then heated up again, the content of the Austenitic phase at T_1 is larger than the Eq. (5) would predict for the heating process. We assume that these equations only describe the transformation of a fraction (1 - dA) of the material and the fraction dA remains in the Austenitic phase. Thus, we set for the history dependent A-phase $R_{A,Hyst}$:

$$R_{A,Hyst}(T) = R_A(T)\,(1 - dA) + dA \quad (10)$$

At temperature T_1, $R_{A,Hyst}(T_1) = R_{A,down}(T_1)$, where the notation down indicates that R_A is calculated with the corresponding values for the cooling process. Using this relation the fraction dA becomes:

$$dA = (R_{A,down}(T_1) - R_{A,}(T_1)) / (1 - R_{A,}(T_1)) \quad (12)$$

The history dependent M-phase is calculated by:

$$R_{M,Hyst}(T) = 1 - R_{A,Hyst}(T)$$

A similar argument holds, if the material is heated up to a temperature $T_2 < A_F$ and then cooled down. In this case Eq. (5) is applied for a fraction (1-dM) of the material. Now, the values for k and T_0 of the cooling process must be used except for $R_{M,up}$(T2).:

$$R_{M,Hyst}(T) = R_M(T)\,(1 - dM) + dM \quad (13)$$

$$dM = (R_{M,up}(T_2) - R_{M,}(T_2)) / (1 - R_{M,}(T_2)) \quad (14)$$

In a history dependent calculation dA or dM are calculated at T_1 or T_2 from the stored values of R_A and $\{\sigma\}$.

3 COUPLING SCHEME

All calculations described in section 2 are automatically controlled by an overlaying program as shown in Fig.2. It launches the programs according to the sequence listed in its input file. The program "Script_tosca" updates mesh datas and transfers results between the other programs. This is controlled by simple commands contained in the input file. At each call to "Script_tosca" the "Regie" program passes the commands to perform the special tasks mentioned above. The execution sequence may be repeated to feed back mechanical data in order to take into account nonlinear effects like stress dependence of the electrical resistance. To control time-dependent calculations, each sequence has an individual time.

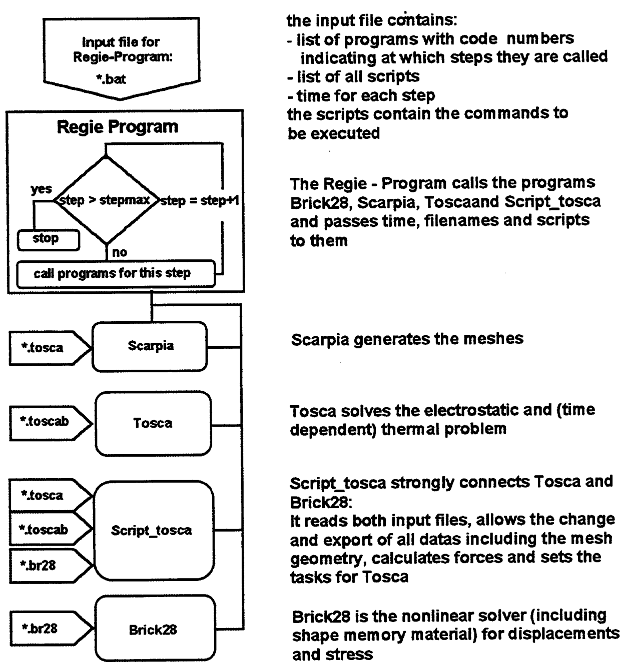

Figure **2**: Simulation scheme for the SMA actuators.

4 SIMULATION RESULTS

In the following the simulation model is applied to two different SMA devices.

4.1 Double Beam Cantilever

The calculated deflection of a double beam cantilever is plotted in Fig.3 as function of homogeneous beam temperatures. The thickness of the beam is 0.096 mm. The dimension in the x-y plane and the simulation parameters are shown in Fig. 3. At x=0 the beam is fixed by a mechanical support. A load F of 2 mN is applied in -z-direction at x=4. In Fig 4 calculated and measured deflections of a dounle beam made of NiTiCu are compared for different temperatures. In this case the simulation parameter are:

E_M = 6.2 GPa, E_A = 70 GPa, σ_{eM} = 20 MPa, F = 10 mN. The phase transition temperatures are determined by differential scanning calorimetry: A_S = 62 °C, A_F = 80 ° C, M_S = 55°C, M_F = 43 ° C.

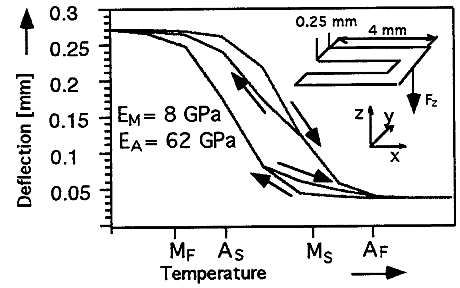

Figure. 3: Beam deflection as function of temperature. Heating and cooling directions are indicated by arrows.

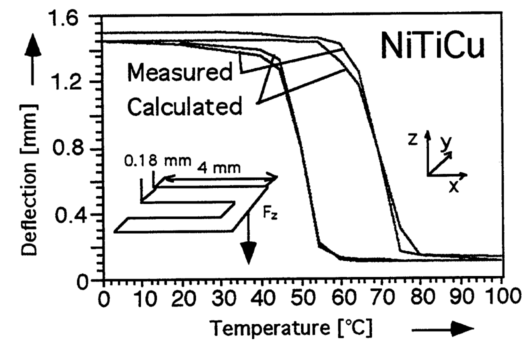

Figure 4: Beam deflection as function of current density

1.2 Double Beam Cantilever

A schematic of the microvalve developed at IMT [7] is shown in Fig. 5. The main components are a plastic housing with an integrated valve seat, a polyimide membrane, a spacer, a SMA microdevice made of NiTi and a cover. As long as no heating current is applied to the SMA microdevice the valve stays in a normaly-open condition. By heating the SMA device above the phase transition temperature the valve is closed by pressing the membrane onto the valve seat. The thickness of the microbridge is 20 µm, the length is 2 mm. The thickness of the spacer is 60 µm. Between the SMA and the cover is a thin isolating layer not shown in Fig. 5. This layer was taken into account for the electrical and thermal calculations. The NiTi material displays a rhombohedral (R-) phase transformation above room temperatur, which is characterized by a narrow hysteresis width of about 1 K. The formalism given in section 2.3 is applied for the R-phase instead of the M-phase. The simulation parameters are listed in Table 1. Fig. 6 shows a series of temperature distributions along the top surface of the SMA microdevice and a horizontal section of the valve cover for different heating times. Due to symmetry, only one half of the device

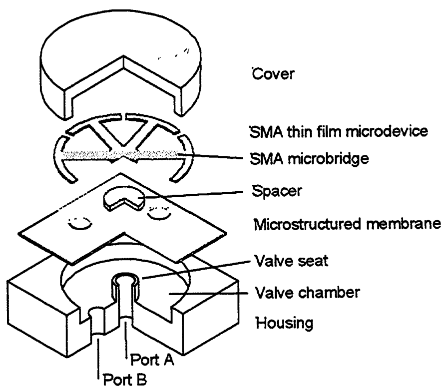

Figure 5: Exploded view of the SMA microvalve.

	NiTi device	Isolator	Cover
Thermal conductivity λ ($Wm^{-1}K^{-1}$)	18.0	0.02	380
Electrical conductivity σ ($\Omega^{-1}m^{-1}$)	$1.2\cdot10^{6}$	0.5	$50\cdot10^{6}$
Specific heat c_p ($Jkg^{-1}K^{-1}$)	450	200	385
Mass density (kgm^{-3})	$6.5\cdot10^{3}$	$4\cdot10^{3}$	$8.8\cdot10^{3}$
Thermal expansion Coeff.icient (K^{-1})	10^{-5}	$6\cdot10^{-5}$	$1.7\cdot10^{-5}$
Heat transfer coeff. $\bar{K}$	70 $Wm^{-2}K^{-1}$		
Integral latent heat of R-phase transformation	450 Jkg^{-1}		
Environment temperature T_E	25 °C		
R_S, R_F, A_S, A_F (°C)	44.0, 25.0, 26.0 ,46.0		
E_A, E_R (Mpa)	62000, 27000		
σ_{eM} (Mpa) , ε_T ,c (K/Mpa)	100.0, 0.06, 0.16		

Table 1: Simulation parameters for the SMA devices

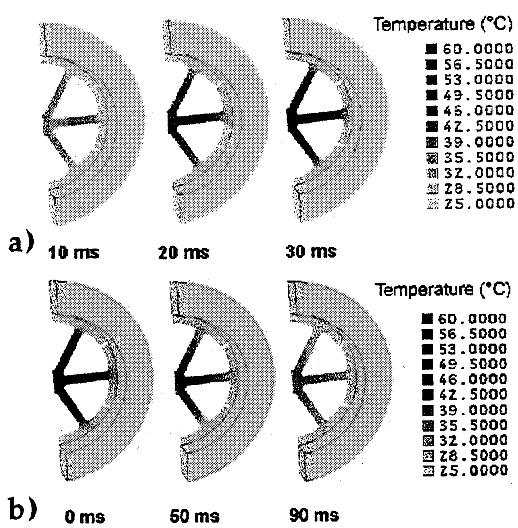

Figure 6: Temperature distributions along the top surface of the SMA microdevice during heating (a) and cooling (b). The time intervals of heating and cooling are indicated.

has been simulated. The electrical power is 85 mW. The temperature distribution along the surface of the microbridges is almost homogeneous except the transition regions close to the bond pads of the SMA microdevice. Within a heating time interval between 25 and 30 ms, more than 95% of the SMA microbridges are heated above the A_F –temperature. Thus, all active regions contribute simultaneously to the closing of the valve. The cooling time is about 90 ms. The results agree well with the measured closing and opening times of 25 and 100 ms. Fig. 7 shows the stress distribution in the mid plain of the SMA microbridge for two heating current densities. At 1 A/mm^2 the maximum stress values are found in the region of the valve where the maximum temperature is 28.2 °C and the A-phase begins to form. At 6 A/mm2 the whole microbridge is in the A-phase and the maximum stress values are found in the region between the microbridge and the surrounding ring structure. The closing force of the valve is determined by the homogeneously distributed stress value in the microbridge, which is 157 MPa at 1 A/mm^2 and 295 MPa at 6 A /mm^2. Experiments show that this valve controls pressure differences up to 5000 hPa.

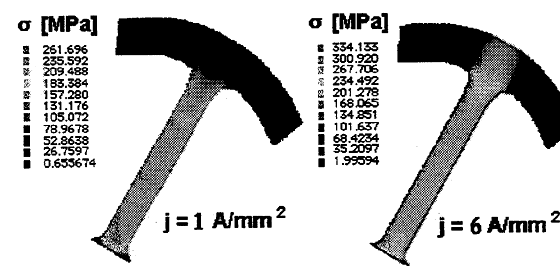

Figure 7: Stress in the mid plain of the SMA microbridge.

5 CONCLUSION

A program package was developed which enables the direct calculation of stresses and displacements of complicated structures of SMAs by coupling of FEM programs. The thermal model and the shape memory model are suitable to verify the experimental results.

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