Finite-element-simulations of polycrystalline shape memory alloys

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ABSTRACT

Paper presents preliminary findings on porting the Mueller-Achenbach-Seelecke model for the constitutive behavior of shape memory alloys into the finite-element-program ABAQUS. Means to doublecheck the current status of the implementation are traced out and the need for thermomechanical coupling in modeling shape memory alloys is demonstrated.

Keywords: shape memory alloys, thermomechanical coupling, single crystal, polycrystal, parameterization, simulation, ABAQUS

1. INTRODUCTION

Shape memory alloys (SMA) are widely employed as sensors and actuators. The need for precise control requires reliable modeling techniques involving, e.g., prescribed stresses and temperatures. These parameters are always inherently coupled in SMA. Various models are in use to characterize the non-linear hysteretic behavior of SMA; among them some that do not provide a means to incorporate true thermomechanical coupling. This aspect is, however, featured by the MAS-model developed by Mueller, Achenbach and Seelecke[1] which is strictly based on thermodynamics. It captures all the salient characteristics of SMA and has already proven its suitability for simulating SMA behavior. The present report portrays preliminary results on the verification of the current implementation of said model in a finite-element-program and its applicability, gives a brief account of the numerical approach and provides an outlook on upcoming work.

2. METHODOLOGY

A FORTRAN implementation of the MAS-model was made available to the author. The MAS-model in its original formulation is strictly applicable only for uniaxial states of stress in single crystals, thereby limiting the loading states that can be addressed by this model. The performance of the model for this load case has been documented before for uniaxial tensile loading[1].

A prime example for uniaxial loading, more sophisticated than purely tensile loading, is the common 'Euler-Bernoulli-beam'- type loading: a straight horizontal cantilever, clamped at one end, is bent by a vertical force acting at the far end. According to theory, the only stress component in the beam is along and parallel to the beam axis.

To verify the present implementation of the MAS-model for single crystals, recourse was taken to the publications of the research group at the North Carolina State University headed by Prof. Seelecke where the cantilever beam was studied in a thesis[2] and analyzed using FEMLAB. The beam is initially in a martensitic state with equal amounts of the variants M+ and M-. The geometry and loading conditions were fed into the finite-element-program ABAQUS (FEM) and results compared. As seen (Fig. 1), the stress varies linearly across the thickness as no phase change has occurred as yet. Under continued loading (Fig. 2), the outer 'fibers' (exposed to higher stresses) are first to experience the phase transformation characterized by a stress plateau and, under yet higher loads, the stresses continue to rise. This profile matches the theoretically predicted stress profile through the thickness[3].

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The simulation also provides equivalent graphs for the phase distribution (Fig. 3). Upon unloading, extremely intricate stress profiles emerge within the beam (Fig. 4). All data considered, good agreement is achieved with the reference solution. However, this FEM simulation is not truly coupled for lack of an adequate element type in the ABAQUS element library: there are no beam elements for thermomechanically coupled problems. Therefore, the procedure type is 'static' and the 'temperature' therein is only a solution-dependent state variable and is thus not accessible as temperature to ABAQUS. The above simulation is hence unable to exploit the capabilities of the MAS model.

To this end, the simple tensile loading of a single crystal SMA wire was once more studied. Two of the three temperature-related terms in the constitutive model, namely the heating caused by an applied electrical current and the heat transfer across the lateral surfaces, were re-written using standard ABAQUS commands for a linearly elastic material and results (prior to any phase changes) juxtaposed to those stemming from the MAS-model (with all simulations using the procedure type 'coupled temperature-displacement'). Good agreement was obtained, corroborating the previous FORTRAN implementation and its interface with ABAQUS. The third and most crucial aspect, the temperature effects caused by phase changes, can however not be verified independently by standard ABAQUS commands.

As single crystals are rarely studied experimentally, the MAS-model was recently extended to polycrystalline SMA using a method labeled 'parameterization'[4]. The approach roots in assumed distributions in barrier stress and interaction stress between individual grains. The technique differs from the single crystal implementation by a transformation stress that varies with the amount of material that has already undergone the transformation; hence requiring a constantly changing stress to drive the deformation further. Hence, the computational simplicity of the single crystal version is formally preserved, even for an arbitrarily large number of crystals. The method results in a smoothly rising resp. decaying transformation stress. Similar to the above approach, own results are close to the ones in this reference and deviations are ascribable to the fact that not all parameters required for the simulations depicted in that reference could be deduced form the graphs therein.

3. RESULTS

The preceding phenomena of thermomechanical coupling and polycrystalline behavior can now be combined in a simulation that more closely resembles realistic experiments. The case studied is once more the tensile loading and unloading of an initially austenitic wire depicted in Fig. 5. The wire is axially stretched in the 'x-direction' till phase changes occur and subsequently unloaded. The phase changes within the material (Fig. 6) cause the temperature to rise. Thermal interaction with the ambiance is by internal heat conduction and convection across the lateral faces. Initially, the specimen is isothermal with the ambiance. A significant thermal gradient is established in the course of the deformation (Fig. 7) between nodes grouped into various node sets (Fig. 5), clearly demonstrating the need for spatial discretization. The thermomechanically coupled computation is able to pinpoint temperatures since temperatures therein are nodal quantities whereas the solution-dependent state variable in the 'static' simulations are element quantities, thereby sacrificing spatial resolution. The stress-strain curve is shown in Fig. 8.

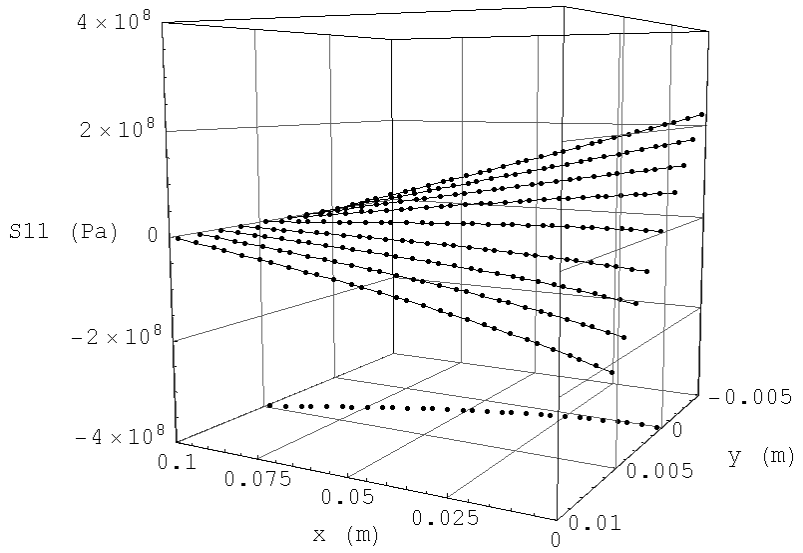

Fig. 1. Simulation of a straight cantilever beam bent by a force acting in the y-direction at x = 0.1 m. Stress on and parallel to the beam axis as a function of spatial coordinates at approx. 0.2 s for Fig. 3.49[2]. Original beam dimensions: Length = 0.1 m, thickness = 0.01 m. The spatial resolution through the beam thickness is provided by section points equidistant through the thickness. The black dots on the base plane provide a graphical impression of the current configuration.

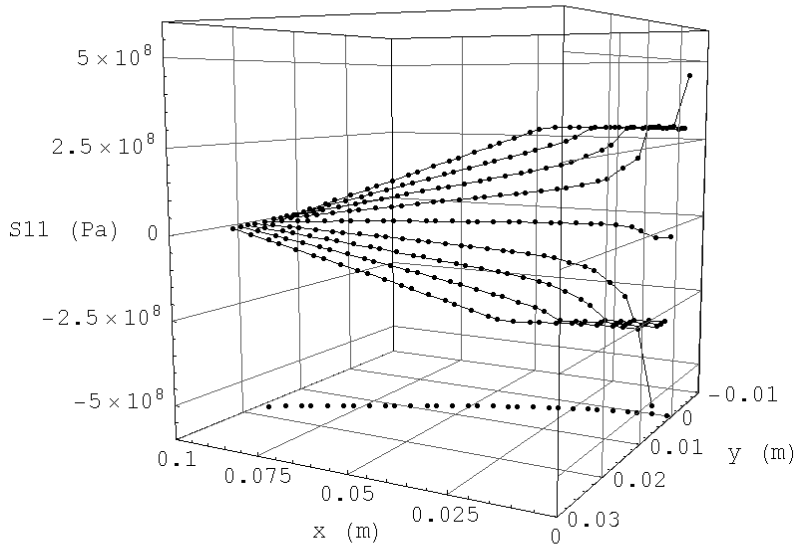

Fig. 2. As Fig. 1, but at approx. 0.4 sec. The stress in outer fibers has reached the transformation stress.

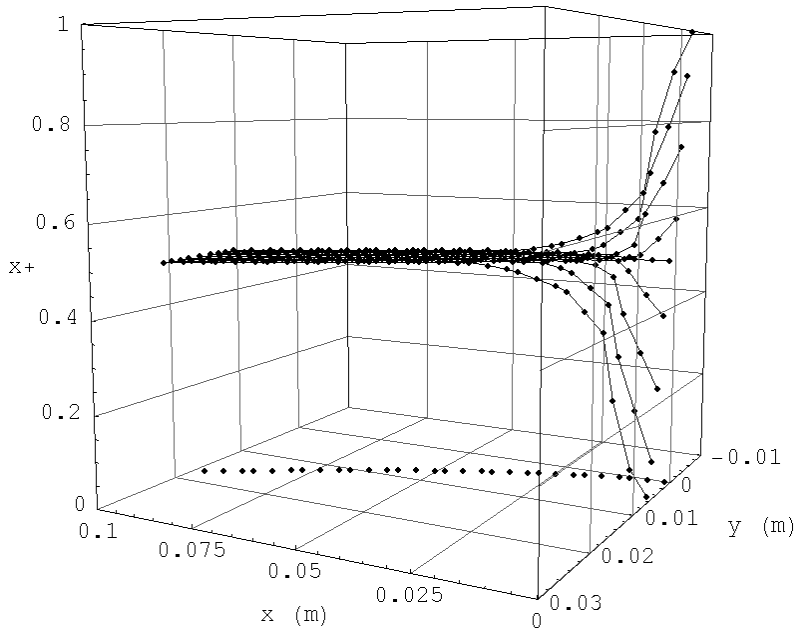

Fig. 3. Spatial distribution of the M+ phase content associated with the stress state in Fig. 2.

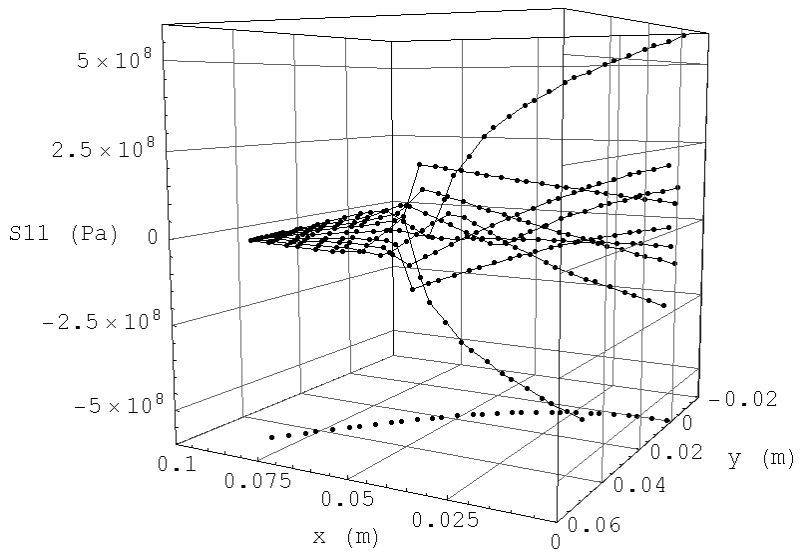

Fig. 4. Same as Fig. 1, but during unloading.

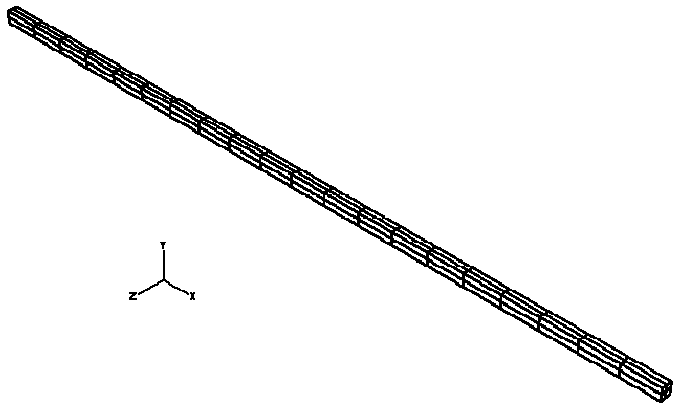

Fig. 5. Wire of a polycrystalline SMA in a simulation. Length: 0.0635 m, height: 1.07 mm, thickness: 0.84 mm. Subsequent figures refer to the following node sets along the x-direction: 'edge' = nodes at an edge, 'face center' = nodes at a face center, 'center' = nodes in the center of the wire.

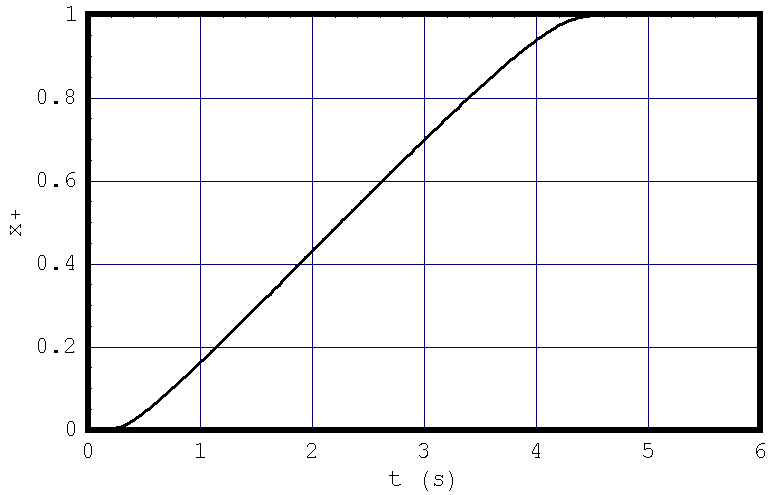

Fig. 6. Phase change in the simulation shown in Fig. 5: temporal evolution of the content in M+ in one volume element; initial configuration purely austenitic.

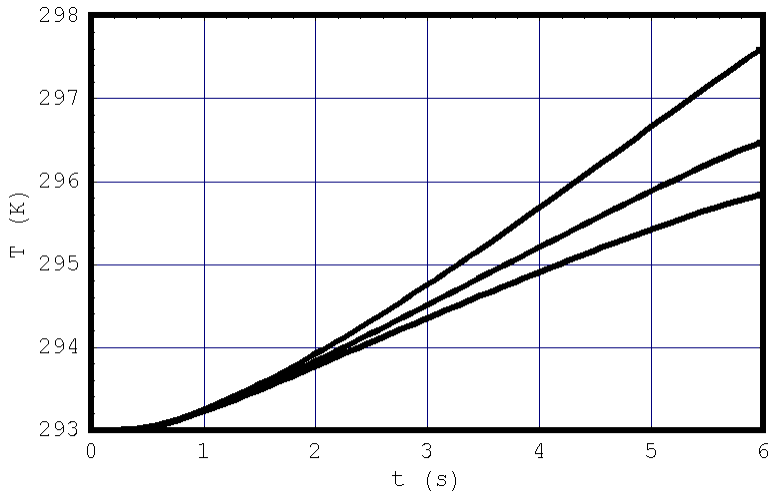

Fig. 7. Temperature as a function of time for various node sets shown in the simulation from Fig. 5 (fully coupled thermomechanical case): highest temperature = 'center', intermediate temperature = 'face center', lowest temperature = 'edge'. The loading gives rise to a thermal gradient of almost 2 K through the thickness of the wire when the maximum strain is attained.

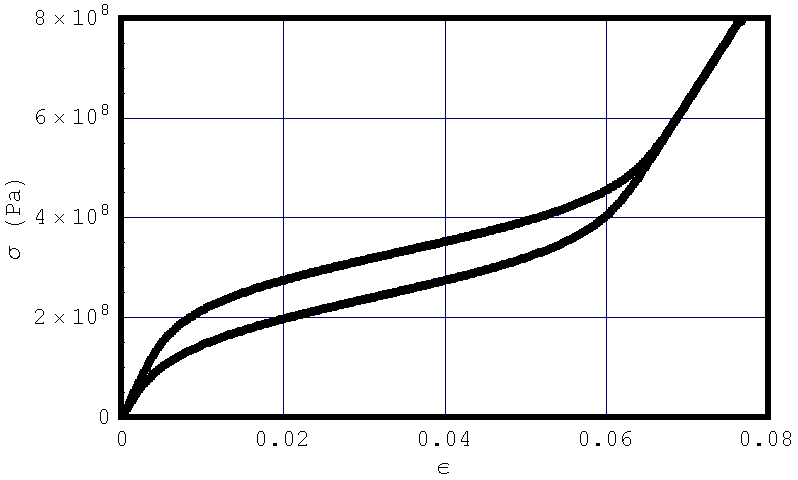

Fig. 8. Stress as a function of strain for the simulation shown in Fig. 5: ‘parameterized’ simulation.

4. CONCLUSIONS

In a first step to using numerical tools for SMA modeling, a FORTRAN program was coded for the ABAQUS UMAT (user material) subroutine and results validated against literature data and, when limited to the initial stage before any phase change occurs, also against standard ABAQUS commands. The output generated with the current implementation of the MAS-model in the FEM program ABAQUS is in consistent agreement with data obtained previously by either the stand-alone FORTRAN program, standard ABAQUS commands or alternative numerical techniques for both single crystals and polycrystals under uniaxial tensile loading. It can thus be stated that the current implementation in ABAQUS is equivalent to all reference data, but makes use of all the advantages of FEM.

An example of simple uniaxial loading of a SMA wire demonstrates that temperature gradients can arise even within a small volume in case of a fast loading rate. Hence, data from the standalone FORTRAN program may only represent a volume average of the amount of net heating.

5. OUTLOOK

The MAS model was derived from fundamental thermodynamic principles, offers explanations of all relevant effects in shape memory alloys and is thus attractive for continued research. Its comprehensive approach along with an expertise accumulated over several years, both theoretical and numerical, will render it even more attractive to users outside the academia where the ever growing interest in the field of smart materials is likely to increase the need for reliable modeling and control tools.

The successful verification of the ABAQUS implementation of the MAS-model now allows focussing on simulating realistic experiments aimed at matching measured data resp. establishing appropriate material constants from available data.

As ABAQUS is a general-purpose FEM package, it provides a vast amount of possible loading scenarios: in contrast to the FORTRAN program, large assemblies of SMA, also with more intricate interaction with its surroundings like non-constant external temperature and arbitrary mechanical loads, even when exerted over only a part of the model, can be reliably computed. Likewise, actuation by an electrical current with oscillating amplitude poses no obstacle. In this aspect, modeling with FEM to arbitrary complexity combined with extended postprocessing options allows to overcome the limitations of the basic FORTRAN program. Even though this code is still at the core of the UMAT subroutine, the code is now called for every 'integration point' within the volume individually and is hence able to resolve the interaction between regions of the model that are exposed to different loads, initial or boundary conditions. Consequently, the precision of the results will rise with the computational effort when requesting high resolution.

Once accomplished, yet another step is projected that will allow to extend the MAS-model to multiaxial states of stress in single crystals[5], also for thermomechanically coupled loading, thereby widening the field of applicability of the model while retaining the benefits of resolution in time and space. In summary, the theory related to the model is already available in condensed form in the literature and the only task left is in programming an appropriate interface with ABAQUS.

The long-time aim is to provide a model for SMA that is capable of both temporal and spatial resolution to any desired degree for virtually any loading case, be it uni- or multiaxial in single crystals or polycrystals, in order to obtain information on the response of the SMA with regard to all quantities of relevance with respect to SMA like the stress and deformation tensors, the flow of thermal energy, phase distribution, latent heat and work output.

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