Implementation of the Müller - Achenbach - Seelecke model for shape memory alloys in ABAQUS

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Abstract: Temperature changes caused by latent phase transformation heats are an integral part of the behavior of shape memory alloys. Among the models capable of incorporating the according thermomechanical coupling between the mechanical and thermal constitutive equations is the one named after Müller, Achenbach and Seelecke. Its versatility when implemented as a standalone program has already been documented for single crystals under uniaxial loading. This code was ported into the 'user material' interface in the commercial finite element package ABAQUS and results validated by comparison with reference solutions. Further, a more recent extension of the model to uniaxially stretched polycrystalline materials was tackled as these are of greater relevance. The approach roots in the method of 'parameterization' which interprets a polycrystal deformation as being equivalent to the one of a single crystal exposed to constantly varying energy barriers. The computational effort of the single crystal version therefore prevails. Thermal gradients can be spatially resolved even in a small volume.

Key words: shape memory alloy, Müller-Achenbach-Seelecke model, thermomechanical coupling, simulation, ABAQUS, beam bending, parameterization

1 Introduction

Shape memory alloys (SMA) are increasingly being employed as sensors and actuators. To assign them a function their behavior should be accessible to physical interpretation to utmost precision, hence reliable modeling techniques are mandatory. Depending on temperature, the constitutive behavior of SMAs is characterized by either pseudoplasticity (at low temperature) or by pseudoelasticity (at high temperature). Ideally, the constitutive model for a SMA should be so versatile as to be able to capture both pseudoplasticity and pseudoelasticity; hence accessing the entire range of SMA behavior. What is more, it is required to model the complex, non-linear hysteretic and thermomechanically coupled material behavior of SMAs. Thermomechanical coupling is inherent to SMA applications as phase changes are inevitably accompanied by temperature effects caused by latent heat. Consequently, mechanical and thermal equations need to be solved simultaneously. A model capable of this truly thermomechanically coupled approach is the one named after Müller, Achenbach and Seelecke (Ref 1, henceforth 'MAS model') which reflects all the salient characteristics of SMA. The majority of the study considers single crystals as their stress-strain curve features a theoretically constant transformation stress, allowing to assess the stress evolution by comparison to the case of an ideally elastic-plastic material. The present publication summarizes results of the implementation of this model in the FEM (Finite-Element-method) environment ABAQUS® (ABAQUS, Inc., Dassault Systèmes, Providence, Rhode Island, USA), indicating harmony to reference solutions taken either from alternative implementations of the model or from basic mechanics.

2 MAS model

Crystallographic observations have revealed that a SMA under uniaxial loading forms a layered structure, each mesoscopic layer being in the phases austenite or variants of martensite. The derivation of the MAS model adheres strictly to thermodynamics and roots in the idea of a three-well potential energy with minima indicating the stable locations of these three phases, austenite (A) and two martensitic twin phases (M+, M-). The preferred modification of martensite is dictated by the direction of stress. Thermodynamical considerations allow to establish a coupled system of three ODE rate equations for the three phase fractions. The temperature evolution within the specimen, taking proper account of latent heat emission and absorption by phase changes, is accompanied by heat convection on external surfaces. Joule heating by an electrical current may be incorporated. The temperature is calculated from the energy balance which represents a fourth differential equation. The resulting 4d-ODE system can be solved numerically. An online version of the model applied to a SMA wire is available for illustrative purposes (Ref 2). As of now, the model has been worked out exclusively for uniaxial states of stress.

3 Numerical implementation

An implementation of the MAS model as a standalone program has been developed and thoroughly tested over several years (Ref 3, Ref 4). This program code was interfaced with the ABAQUS subroutine UMAT (User Material) but is now called for every 'integration point' within the volume individually. Thus, the present version features the following major advantages as opposed to the previous program: the deformation is no longer limited to tension, the geometry and spatial discretization are arbitrary, internal heat conduction generates thermal gradients, mechanical and thermal interaction with other parts of the model and the ambiance can be incorporated. The phase fractions and the temperature enter as solution-dependent state variables (SDV). Unless specific instructions are incorporated within the UMAT, these quantities remain without physical significance to ABAQUS. Thermomechanical coupling is achieved upon ascribing the fourth SDV to the ABAQUS variable RPL within UMAT. Note that not all of the regular ABAQUS element types are capable of this coupling; some elements used in this work are strictly mechanical. In this case the temperature is held constant. At the current level of sophistication, verification of FEM results is restricted to close reproduction of the outcome of the stand-alone program and an implementation in FEMLAB® (COMSOL AB, Stockholm, Sweden, Ref 5).

4 Results

4.1 Beam bending

Beam bending is somewhat more sophisticated than simple tension as the magnitude and the sign of the uniaxial stress varies through the thickness. Planar Euler-Bernoulli beam elements are attractive as they feature a single stress and strain component along and parallel to the beam axis. However, the ABAQUS element library does not offer a beam element for coupled temperature-displacement procedures. All simulations dealing with beam elements are therefore strictly isothermal, excluding latent heat, internal heat conduction and heat transfer across the external surfaces. All simulations in this section incorporate geometrically nonlinear behavior and model the beam using the ABAQUS Euler-Bernoulli-beam element B23. The capability of the MAS model in simulating the behavior of SMA single crystals in beam bending is demonstrated by the independent examples in the sequel.

a) The bending of a straight horizontal cantilever fully restrained at one end and loaded by a vertical point force at its free end has been analyzed before (Ref 5). The force is defined as a follower load and the constitutive behavior is pseudoplastic with initially equal fractions of M+ and M-. A representative result is depicted in Fig. 1 showing the profile of the M+ fraction over the cross-section of the beam in three-dimensional space at the instant of maximum deflection. Upon bending, the solution exhibits the typical compression/tension profile of stress for Euler-Bernoulli beams in the elastic regime modulated by pseudoplastic/pseudoelastic behavior in the transformation regime (Ref 6). Accordingly, the phase fractions of the martensitic variants evolve along the cantilever. The M+ fraction increases in the tension regime below the neutral fiber whereas above it the M- fraction is growing at the expense of the M+ fraction. The neutral fiber is indicated by the feet of the respective data points on the (x,y)-plane, showing the actual deflection in this plane.

Analogous graphs can be constructed for the M- fraction, the stress and the strain. Such load-induced phase changes and the according formation of martensite plates has been verified experimentally for polycrystalline beams (Ref 7).

b) An analytical solution of the plastic zone can be computed for vertically loaded cantilevers for the special case of an ideal elastic-plastic constitutive relation (Ref 8). This solution can be compared to the deformation field of a pseudoplastic SMA cantilever produced by the FEM-embedded MAS model as shown in Fig. 2. Both theories predict the same boundary line of the plastic zone (solid black line in Fig. 2) thus verifying the numerical validity of the computer model. Note that the analytical solution is capable of this boundary line only while the MAS model additionally provides the concentration field of the M+ phase. Both solutions were calculated on the basis of the geometrically nonlinear theories.

4.2 Torsion of a pseudoelastic SMA tube

Conveniently, torsion is characterized by a uniaxial state of stress and thus accessible to the MAS model. The free oscillation of a pseudoelastic SMA pendulum at constant temperature (T=353 K) has been studied in Ref 9 and Ref 10 using the standalone implementation of the MAS model. We adopt the setting from Ref 9 to study the behavior of the FEM based computer model where the earlier results serve as reference solution. The torsion pendulum is represented by a thin-walled pseudoelastic NiTi tube (2 mm diameter, 5 cm length, 50 µm wall thickness). Supported at one end, this tube is attached to a weight at the opposite end which produces the required inertia upon free oscillation. The oscillation started from a pre-twisted state where the according torque induces a pure martensitic state. In the FEM based computer model the tube is discretized by 10 ABAQUS beam B33 elements along the axis. The FEM based solution and the reference solution are juxtaposed in Fig. 3 where the black dots indicate the reference solution and lines reflect the FEM based torsion at three axial nodes (located at the tube ends and in the center, respectively) as function of time. The reference solution coincides with the torsion/time function of the node at the tube end. At the center node the torsion is proportionally less while the fixed node remains at rest. During the first 50 s the inertia of the weight produces sufficient torque to loop the material through the pseudoelastic hysteresis. Accordingly, hysteresis-related energy dissipation causes the significant damping visible in Fig. 3. Eventually the material behaves purely elastic, affecting undamped harmonic oscillations.

4.3 Tensile test of a polycrystalline SMA wire

Seelecke and Heintze (Ref 11, Ref 12) have contributed a polycrystalline formulation of the MAS model which overcomes some of the physical limitations of the originally single-crystalline model. The method of ‘parameterization’ renders the model more flexible but preserves the computational simplicity of the single crystal implementation with minor adaptations. The polycrystal model takes into account the averaged excess stresses occuring in a domain-structured material (originating from grain orientations, local transformation stresses and other local effects). It has been ported into the ABAQUS environment and was used to simulate uniaxial straining of a pseudoelastic SMA wire. The results are compared to the literature (Ref 11). The FEM model employs the ABAQUS element type C3D8T to discretize a wire into 8x8x4 (width x thickness x length) elements. This element type is capable of 3D problems, but for the special case of uniaxial loading the application of the one-dimensional polycrystalline MAS model is possible. The significant advantage of the C3D8T element over the formerly used beam-type elements is that this element type permits true thermomechanical coupling. Fig. 4 and Fig. 5 show the result of such a tensile test with a tetragonal wire geometry. The wire is loaded and unloaded in displacement control mode so as to simulate a complete pseudoelastic loading cycle, see inset in Fig. 4. Temperature effects occur during yielding (0-6 s) and recovery (100-106 s) of the transformation strain (see Fig. 4, inset), where the release and the absorption of latent transformation heat affects self heating and self cooling, respectively. These effects are compensated by heat exchange with an ambient medium at a temperature of 293 K. The temperature profile resulting from these heat transfers can be resolved in the simulation: Fig. 5 shows a contour plot of the temperature field at the tip face of the wire for the situation of the fully transformed wire at maximum load (after 6 s). Note the minute thermal conductivity was chosen deliberately to create a notable thermal gradient throughout the tiny volume of the wire. Fig. 4 shows the temperature evolution at three nodes sets localized along the volume center, a face center and an edge of the wire. Because the local temperature deviations are small in a wire geometry, the resulting stress-strain curve for all elements matches the one digitized from the reference (Fig. 6).

Conclusions

Evaluating the results presented, it can be stated that the ABAQUS-version of the MAS model is capable of achieving a good match to digitized data from reference solutions or, where applicable, analytical computations from within the UMAT interface of ABAQUS. Numerics is strongly influenced by various settings including mesh refinement, time incrementation etc. and it must be borne in mind that the computation necessitates a number of tolerances that are not indicated in the reference solutions.

In summary, it can be safely stated that the MAS model is well suited to describe the constitutive behavior of SMA, be it for single crystals or for polycrystals. A prime advantage is its versatility, including the inherent thermomechanical coupling and the extension to polycrystalline materials.

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Figure captions

Fig. 1: Spatial distribution of the martensite M+ phase in a cantilever under vertical loading. The straight cantilever is clamped at x=0 in the pseudoplastic state and bent by an external force acting in the y-direction at x = 0.1 m. Plotted is the spatial distribution of the M+ phase content on and parallel to the beam axis as a function of spatial coordinates at the instant of maximum bending. The spatial resolution through the beam thickness is provided by section points equidistant through the thickness. The black dots on the base plane show the beam curvature. Original beam dimensions: Length = 0.1 m, thickness = 0.01 m (Ref 5).

Fig. 2: Contour plot of the M+ fraction (plotted on the undeformed configuration; only 30% of the beam from the clamped end are depicted), defining the transformation zone in a pseudoplastic cantilever at vertical tip loading in the positive y-direction. The load equals 1.825 times the yield load as detected for the geometrically linear case. The black solid line indicates the analytical solution for the plastic deformation boundary obtained from an ideally elastic-plastic material (digitized from Ref 8).

Fig. 3: Free oscillation of a pseudoelastic NiTi torsion pendulum. Comparison of a reference solution from the literature (black dots, Fig. 3 in Ref 9) with the FEM-embedded version of the MAS model (colored lines). Initially the pendulum is twisted by 324°. Red lined: Fixed tube end (no angular displacement), blue line: node at mid-length, green line: torqued end.

The reference solution refers to the latter; the red and blue solutions illustrate the axial evolution of the torsion.

Fig. 4: Temperature as a function of time for three node sets located at the volume center (solid line), face center (dashed line) and edge (dotted line). Inset: imposed strain as function of time.

Fig. 5: Contour plot of the temperature field (‘NT11’, in K) at the tip of the fully transformed wire at maximum load (after 6 s in Fig. 4), showing a pronounced temperature gradient which indicates the internal heat flux.

Fig. 6: Simulated stress/strain curve of a pseudoelastic, tetragonal SMA wire under uniaxial straining. Black dots: FEM based simulation, squares: reference solution taken from the literature (Fig. 4.11 in Ref 11).

Figures

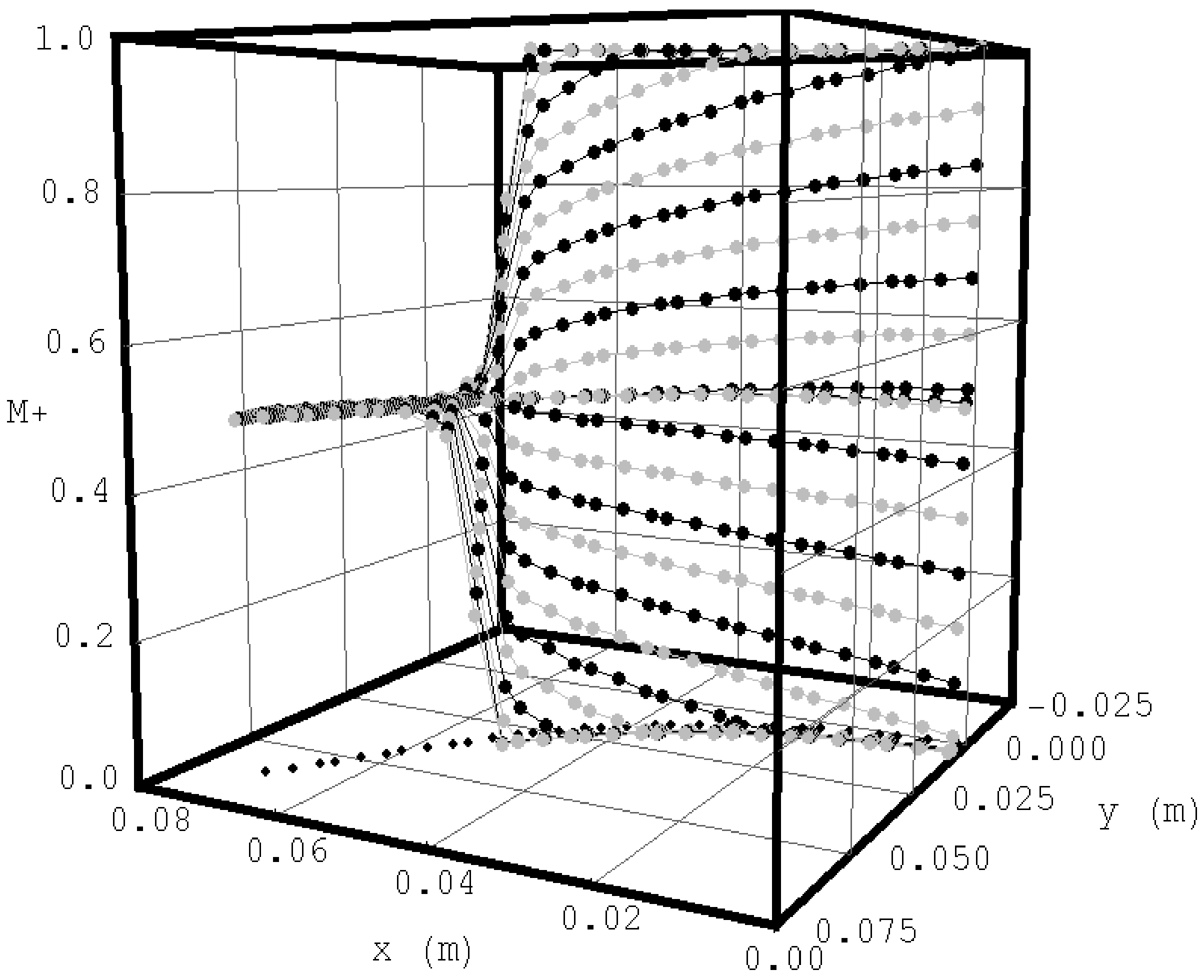
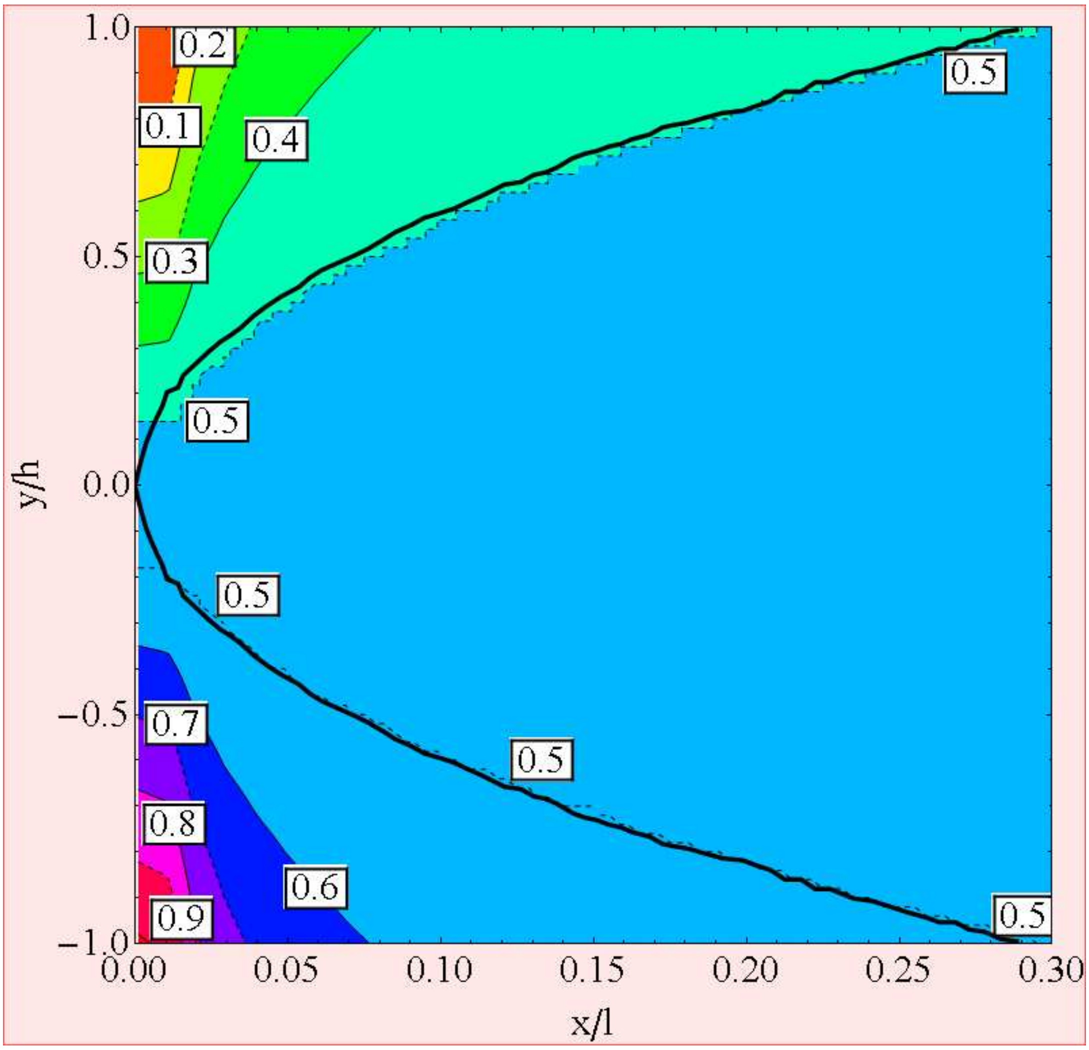


Fig. 1



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0.2
0.3
0.4
0.5
0.5
0.5
0.5
0.5
0.6
0.7
0.8
0.9
y/h
x/l
1.0
0.5
0.0
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0.10
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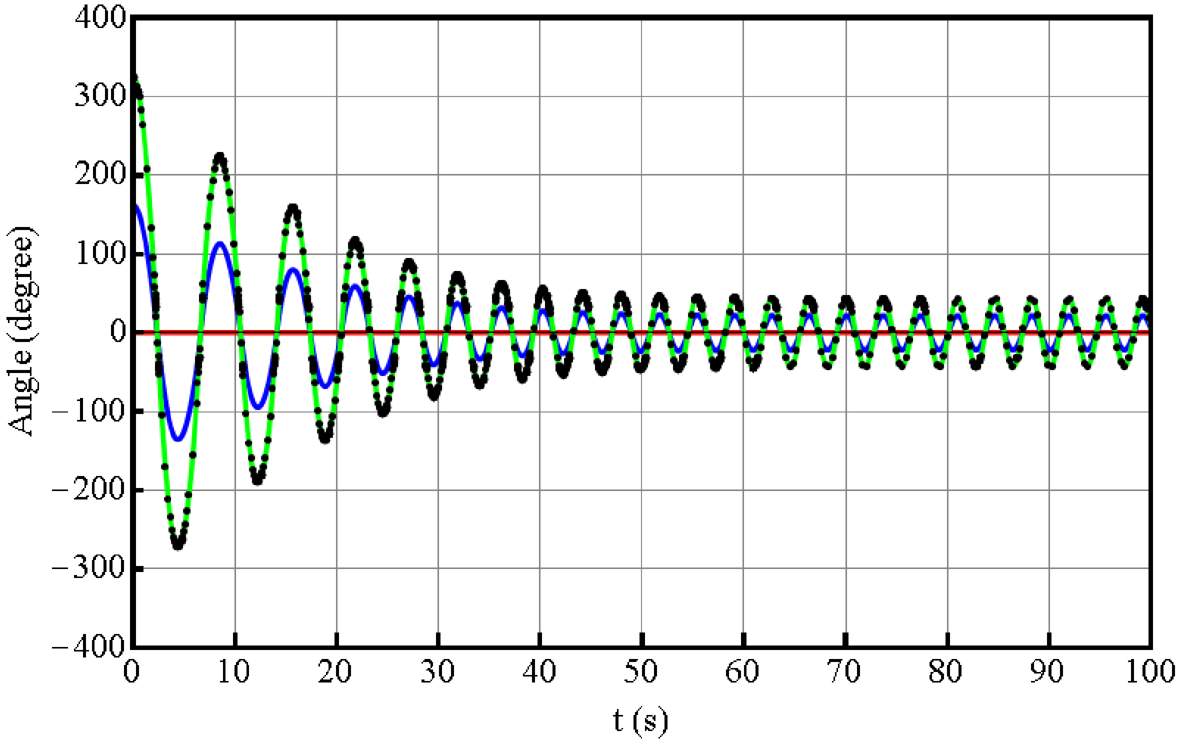
0.30

Fig. 2



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0
−100
−200
−300
−400
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20
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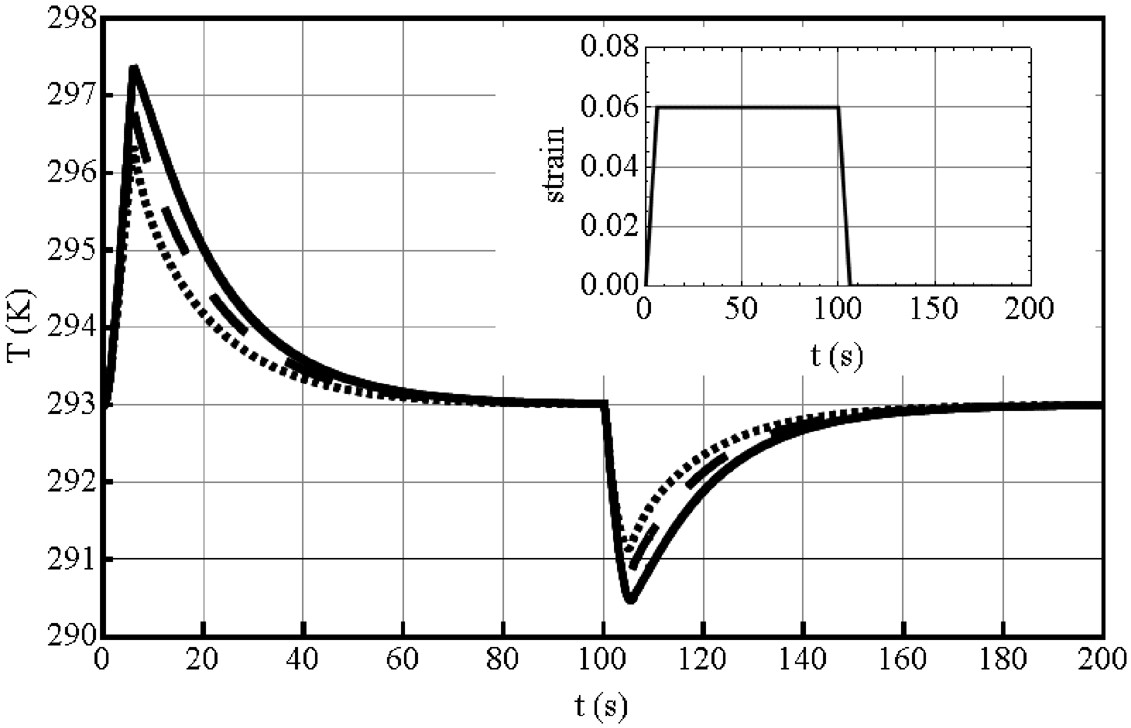
40
50
60
70
80
90
100
t (s)

Fig. 3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180
200
t (s)
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0.04
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strain
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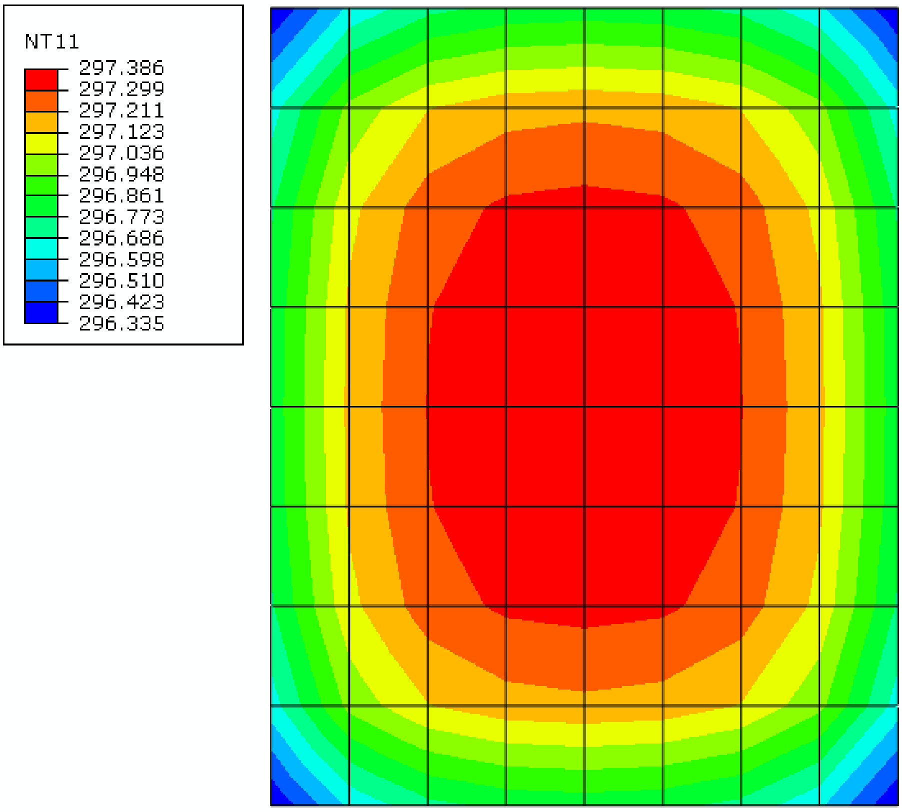
50
100
150
200
t (s)

Fig. 4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296.335

Fig. 5

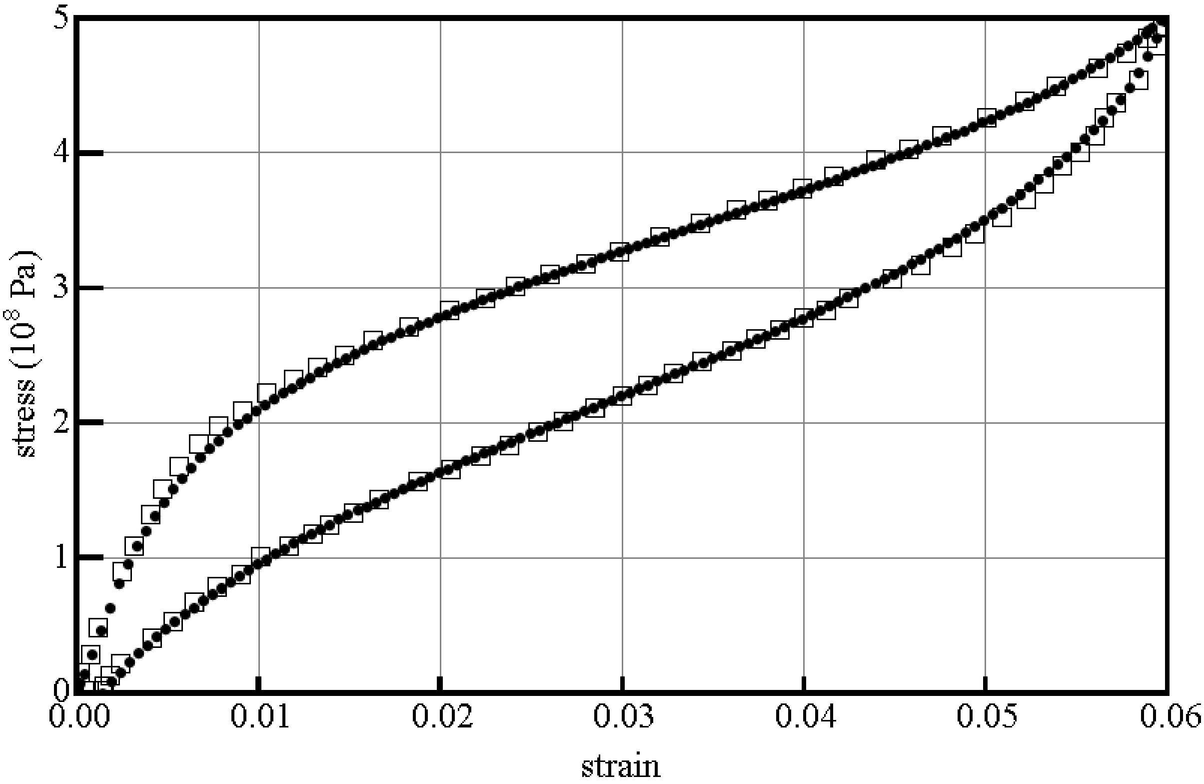

Fig. 6

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