Dynamic Simulation for Hysteresis in Shape Memory Alloy under Tension *

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We demonstrate that the Suliciu model is capable to model the hysteresis phenomenon observed experimentally in NiTi shape memory alloy micro-tubes. This model allows a class of stationary phase interfaces. By a series of fully dynamic numerical simulations that mimic quasi-static loading and unloading, the nominal stress-strain curve exhibits a big hysteresis loop, which quantitatively agrees with the experimental results.

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First-order martensitic phase transition accounts for many interesting physical properties and wide applications of shape memory alloys (SMA).1,2 Although phase transitions are regarded well understood at microscopic level by theories of renormalization group, non-convex free energy, non-monotone structural relation and so on, a macroscopic constitutive description of real polycrystals is far from being fully quantified.3 For instance, an effective modeling is not available for an interesting hysteresis phenomenon observed by Sun et al. in NiTi SMA micro-tubes through careful experimental measurements.4−6 More precisely, they performed a uniaxial tension loading in a quasi-static manner on a NiTi SMA micro-tube. Phase transition occurs in terms of a spiral martensitic band, when the strain exceeds 1.7%. The volume ratio of martensitic band increases along with the loading, while the stress remains basically unchanged. When the micro-tube reaches fully martensitic at a strain around 6%, further increment of loading leads to elastic behaviour with an increasing stress. During the unloading period, the phase transition begins only when the strain reduces to 5.2%. In a later stage of unloading, the martensitic band gradually diminishes, until a linear elasticity is recovered at a strain of about 0.7%. By hysteresis we refer to the different nominal stress-strain curves during the loading and unloading stages. To motivate an explanation, we recall that a non-monotone structural relation results physically in the instability that triggers the transition in SMA, as well as mathematically in the existence of multiple solutions for the governing equations.7 Hence one need include further information or certain mechanisms to identify the true physical processes. For instance, at a phenomenological level, Abeyaratne and Knowles suggested to specify a kinetic relation and a nucleation criterion, both regarded as material properties in addition to the structural relation.8 Under certain contexts, their approach may be shown mathematically robust. Alternatively, one may include dissipation mechanisms to stabilize the transient processes. Such dissipation mechanisms also identify the unique dynamics. Over the past several decades, explorations have been made for high order dissipations, such as a viscosity-capillarity formulation and a mass-viscosity formulation,9,10 as well as for low order dissipations, such as the Suliciu model, a relaxation model, and a more general class of discrete kinetic models.11−14 In the singular limit of zero dissipation, these models yield various kinetic relations and nucleation criteria. It is noticed that most models satisfy the Maxwell construction of equal area law for a stationary phase transition. From a physics argument of free energy minimization, one finds that the stress across such a stationary interface is uniquely determined by the structural relation. However, the Suliciu model violates the Maxwell construction. As we shall see in the following, it actually allows any stationary phase interface provided that the stress keeps the same across it. We remark that for given initial and boundary data, the Suliciu model describes phase transition with a unique dynamics and hence a unique asymptotic stationary profile. However, the asymptotic stationary profile depends on the given initial and boundary data. It is worth mentioning that this property makes the Suliciu model capable to model hysteresis in NiTi SMA. In this Letter, we demonstrate how the Suliciu model faithfully reproduces hysteresis observed experimentally.

First we describe the Suliciu model and some theoretical results. Then we present simulation results that agree very well with the experiments.

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We start with the Suliciu model in one space dimension as follows:

\[ \begin{align*}
\partial_t \varepsilon - \partial_x v &= 0, \\
\rho \partial_t v - \partial_x w &= 0, \\
\partial_t w - E_D \partial_x v &= \frac{\sigma(\varepsilon) - w}{\tau},
\end{align*} \tag{3a,b,c} \]

where \( \varepsilon \) is the strain, \( v \) the velocity, \( \rho \) the density, and \( w \) an intermediate variable. A numerical ‘modulus’ \( E_D \) is chosen suitably big according to a so-called sub-characteristic condition to stabilize the system, and a relaxation time \( \tau \) is chosen as a small parameter.\[16\]

We make a rescaling for the variables as follows:

\[ (t, x, \varepsilon, v, w, \sigma) \to (\eta t, x, \varepsilon, v L/\eta, E^* w, E^* \sigma), \tag{2} \]

where \( L \) is the micro-tube length. We take \( E^* = 10 \text{GPa} \), corresponding to 100 MPa stress for 1% strain. We take a time scale \( \eta = \sqrt{\rho L^2/E^*} \), which is on the order of \( 10^{-8} \text{s} \) for a micro-tube around 0.005 m. Then the non-dimensionalized governing equations become

\[ \begin{align*}
\partial_t \varepsilon - \partial_x v &= 0, \\
\partial_t v - \partial_x w &= 0, \\
\partial_t w - \lambda^2 \partial_x^2 v &= \frac{\sigma(\varepsilon) - w}{\tau}.
\end{align*} \tag{3a,b,c} \]

For the numerical simulations presented here, we take \( \lambda^2 = E_D/E^* = 9, \bar{\tau} = \tau/\eta = 10^{-4} \). By a standard Chapman–Enskog expansion, it may be explained that a smaller \( \lambda \) and a smaller \( \varepsilon \) correspond to less dissipation. The stress is specified by the trilinear structural relation

\[ \sigma(\varepsilon) = \begin{cases} 
\sigma_1/\varepsilon, & \varepsilon < \varepsilon_1, \\
\sigma_1 + (\sigma_2 - \sigma_1)/\varepsilon_1 (\varepsilon - \varepsilon_1), & \varepsilon_1 < \varepsilon < \varepsilon_2, \\
\sigma_2 + (\sigma_3 - \sigma_2)/(\varepsilon - \varepsilon_2), & \varepsilon > \varepsilon_2.
\end{cases} \tag{4} \]

According to the experimental results, we take \( \varepsilon_0 = 0.71\%, \varepsilon_1 = 1.7\%, \varepsilon_2 = 5.2\%, \varepsilon_3 = 6.46\%, \) and \( \sigma_0 = \sigma_2 = 200 \text{MPa} \), \( \sigma_1 = 3\sigma_3 = 480 \text{MPa} \). The austenite phase corresponds to a smaller strain \( \varepsilon < \varepsilon_1 \) and a modulus \( E_A = \sigma_1/\varepsilon_1 \), whereas the martensite phase corresponds to a larger strain \( \varepsilon > \varepsilon_2 \) and a modulus \( E_M = (\sigma_3 - \sigma_2)/(\varepsilon_3 - \varepsilon_2) \). The state between them is unstable, representing the softening of the material with a negative modulus \( E_T = (\sigma_2 - \sigma_1)/(\varepsilon_2 - \varepsilon_1) \).

For a given initial data \( w(x, 0) \), we may rewrite the governing equations (3b)-(3c) in the following form:

\[ \begin{align*}
\partial_t v - w(x, 0) \exp(-t/\bar{\tau}) &- \partial_x \int_0^t \left[ \frac{\sigma(\varepsilon(x, s))}{\tau} \right] ds \\
+ \lambda^2 \partial_x^2 v(x, s) \exp \left( \frac{s-t}{\bar{\tau}} \right) ds &= 0.
\end{align*} \tag{5} \]

We observe that the momentum flux contains memory effects in terms of a time convolution. In the singular limit \( \varepsilon \to 0 \), we recover the standard governing equation

\[ \partial_t \varepsilon - \partial_x v = 0, \quad \partial_t v - \partial_x \sigma(\varepsilon) = 0. \tag{6} \]

As we discussed before, the system (6) does not provide a complete description for the dynamics. In particular, it fails to identify the phase transition dynamics. With the more complete system (3), it may be readily verified that a class of stationary phase interfaces exist in the following form:

\[ (\varepsilon(x, t), v(x, t)) = \begin{cases} 
(\varepsilon_-, 0), & x < x_0, \\
(\varepsilon_+, 0), & x > x_0.
\end{cases} \tag{7} \]

where \( x_0 \) is an arbitrary position, and the strains across the interface lies in different phases, that is, \( 0 < \varepsilon_- < \varepsilon_1, \varepsilon_+ > \varepsilon_2 \), or the other way around. The corresponding stresses are required to be the same constant, namely \( w(x, t) \equiv \sigma(\varepsilon_-) = \sigma(\varepsilon_+) \). Such a stationary phase interface is nonlinearly stable.\[15\]

\[ \text{Fig. 1.} \quad \text{Trilinear structural relation.} \]

In the following, we perform numerical simulations to the Suliciu model (3). We scale the micro-tube length to 1. The left end is fixed. A pulse velocity input \( f(t) \) is loaded for a duration of \( t_0 \) at the right end, to mimic the quasi-static loading procedure. This leads to a strain increment \( \int_0^{t_0} f(t) \) dt to the micro-tube at each loading step. In the following simulations, we take this increment as 0.002%. In Fig. 2., we depict the transient strain profile for the first loading step. An elastic wave enters the micro-tube from the right, propagates to the left, and is reflected back and forth. After a long run, the strain equilibrates to a constant profile. We terminate the simulation of a loading step when the maximal velocity is less than \( 10^{-9} \). A subsequent pulse input is loaded after the system equilibrates. The unloading simulations are performed in a similar way.

The numerical results are summarized in Fig. 3. We observe that during the quasi-static loading stage,
the micro-tube first behaves in an elastic manner with gradually increasing stress, which is uniform in space. Nucleation begins at a strain around \( \varepsilon_1 \). Beyond this strain, martensitic bands appear with a stress \( \sigma_3 \), which equals to that for the austenitic stress response at strain \( \sigma_1 \). The nominal stress thus remains unchanged, while the average strain may vary between \( \varepsilon_1 \) and \( \varepsilon_3 \). The phase transition saturates at a strain around \( \varepsilon_3 \). Further loading leads to an elastic response of the uniformly martensitic micro-tube. During the unloading stage, however, a uniform martensitic elastic response persists until the strain is smaller than \( \varepsilon_2 \). Austenitic bands nucleates and the volume ratio varies while the average strain decreases gradually from \( \varepsilon_2 \) to \( \varepsilon_0 \). The micro-tube returns to uniformly austenitic at strain \( \varepsilon_0 \), and further decrement in strain yields austenitic elastic response. We plot the experimental measurements by Sun et al. in Fig. 4, for comparison. It is obvious that our numerical results for the Suliciu model quantitatively reproduce the hysteresis.

![Fig. 2. Snapshots of strain profile in one loading step. Time \( t \) is identified on top of each snapshot.](image1)

![Fig. 3. Nominal strain-stress curve by numerical simulations.](image2)

![Fig. 4. Nominal strain-stress curve by experiments (courtesy of Professor Q. P. Sun).](image3)

![Fig. 5. Strain profiles at various loading and unloading stages: (a) uniform austenitic micro-tube with strain 1.4%, (b) loading stage with strain 3%, (c) uniform martensitic micro-tube with strain 6%, (d) unloading stage with strain 3%.](image4)

On the nominal strain-stress curve, we take four representative settings. Settings (a) and (c) are during the austenitic and martensitic elastic responses, respectively. The corresponding strains are 1.4% and 6%. In Figs. 5(a) and 5(c), we observe spatially uniform strain profiles for these two cases. On the other hand, the strain profiles differ at the same nominal strain 3% on the loading and unloading stages, as shown Figs. 5(b) and 5(d). In particular, we observe abrupt phase interfaces, which correspond to the sharp bands observed experimentally in three space dimensions. We remark that the number and precise position of the interfaces depend on the loading history, as well as numerical procedure in simulations. This shares some common features with experimental observations of the sharp martensitic bands, which may depend on the loading history and defects or grain boundaries of the micro-tubes. The nominal strain-stress curve fits well the experimental results, partic-
ularly the hysteresis.

Although the position of phase interfaces depends on loading history and possible perturbations, the volume ratio of the martensitic band may be computed. We know that at a martensitic volume ratio $\alpha$, the average strain is $\varepsilon_a = (1 - \alpha) \varepsilon_1 + \alpha \varepsilon_3$. Consequently, we may compute the volume ratio according to

$$\alpha = \frac{\varepsilon_a - \varepsilon_1}{\varepsilon_3 - \varepsilon_1}. \quad (8)$$

In Fig. 6, we plot the numerically computed volume ratio together with the theoretical prediction (8) during the loading stage. The agreement is satisfactory. We remark that the staircase appearance of the numerical results is an artifact due to the finite grid length. With a finer mesh, the numerical curve becomes smoother, and fits better the theoretical prediction.

![Fig. 6. Martensitic band volume ratio during the loading stage with the dashed line for the theoretical prediction and the solid line for the simulation results.](image)

In summary, we have verified the capability of the Suliciu model for simulating the hysteresis phenomenon observed in NiTi SMA micro-tubes. The numerical results agree with the experimental measurements very well. The memory effect in terms of a convolution for the momentum flux accounts for this capability. It is interesting to remark that the Suliciu model fails to satisfy the Maxwell construction for stationary phase transition, which is well believed to hold for microscopic theory or for bulk material. However, the lack of uniqueness for stationary phase transition profiles enables this model to describe phase transition in SMA micro-tubes. A substantial understanding to the physics of such a model is desirable. We further remark that hysteresis was studied through the Suliciu model in a CuZnAl SMA bar in Ref. [11]. However, they only performed a coupled dynamic-quasistatic simulation, possibly due to the lack of computing power and effective solvers. Their control boundary conditions thus differed from the experimental conditions. No multiple phase interfaces were reported. In contrast, we have performed a fully dynamic simulation with pulse velocity input, which resembles one step of loading or unloading. A series of fully dynamic simulations then mimics the quasistatic loading and unloading. Furthermore, we have observed multiple phase interfaces, which resembles the spiral bands in experiments. Noticing that the current study in one space dimension is not adequate to model some other interesting features of the experiments, we plan to simulate higher space dimensions, aiming at reproduction of the rotating angle for the spiral bands. We are also seeking for an explanation of the stress drop right after the martensitic band nucleation. Furthermore, we remark that the Suliciu model is a macroscopic model without considering interface energy or microstructure in general. It was reported recently that hysteresis may be nicely explored in terms of a multiscale process, including the microstructure information such as the grain size and phase interface thickness.\[17,18\]

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References
