A Model for the Simulation of Shape Memory Behaviour

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Introduction

Structural models of material behaviour have heuristic value, because they promote the understanding of physical phenomena and they permit the simulation of experiments on the computer.

Thus it is with models for pseudoelasticity and shape memory. It is necessary here to identify the energetic and entropic contributions to the free energy that governs the austenitic-martensitic phase transition at high temperature and the martensitic twinning at low temperature.

In this paper we shall describe a model and test it by making it simulate the well-known schematic load-deformation curves of Figure 1 as well as the plots of Figure 2 which are taken from an actual tensile-test on a NiTi specimen.

A reflection on the width of the pseudoelastic hysteresis concludes the paper.

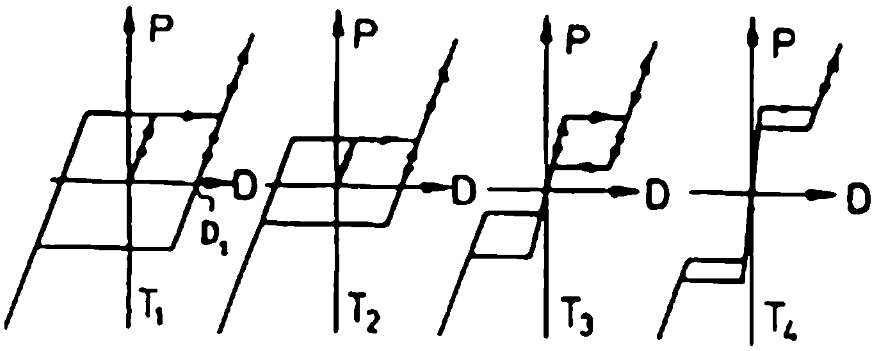

Figure 1: Schematic load-deformation curves for increasing temperatures.

The Model

The basic element of the model is a lattice particle shown in three equilibrium configurations in Figure 3. A denotes the austenitic phase and $M_{\pm}$ are the martensitic twins. We may think of the twins as being sheared versions of the austenitic particle. The curve in Figure 3 shows the postulated form of the potential energy of a lattice particle. It has a metastable minimum for the austenitic phase and stable minima for the twins.

Figure 4 shows how the model body is composed from the lattice particles and how it lengthens and contracts upon loading, heating and cooling. Each layer contributes the vertical component of the shear length Δ to the deformation. Thus, if there are N_Δ layers of shear length Δ, the deformation is equal to

$$D = \frac{1}{\sqrt{2}} \sum_{\Delta} \Delta \, N_\Delta \, , \tag{1}$$

where the summation is over all shear lengths.

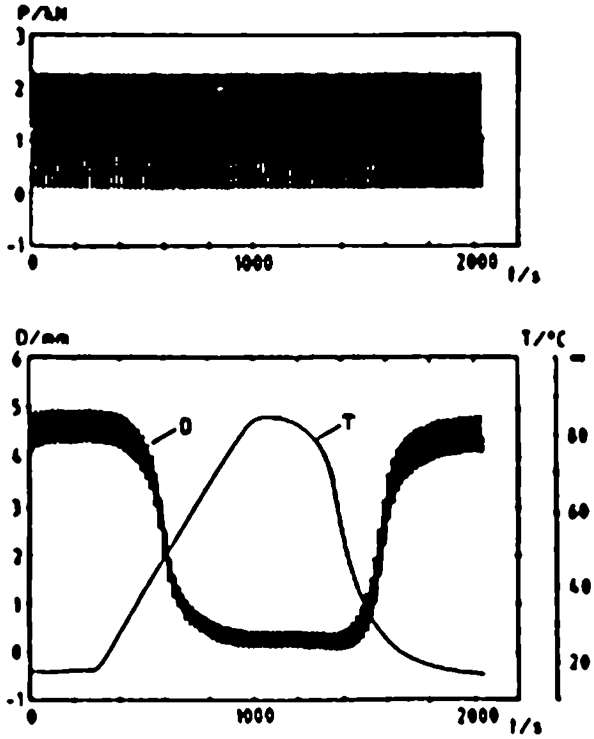

Figure 2: A NiTi specimen is subject to a triangular tensile load and a temperature which first increases and then decreases. The resulting deformation is plotted. [1]

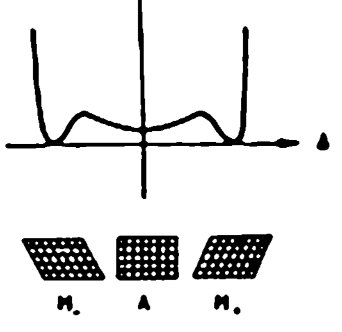

Figure 3: Lattice particle and its potential energy Φ(Δ)

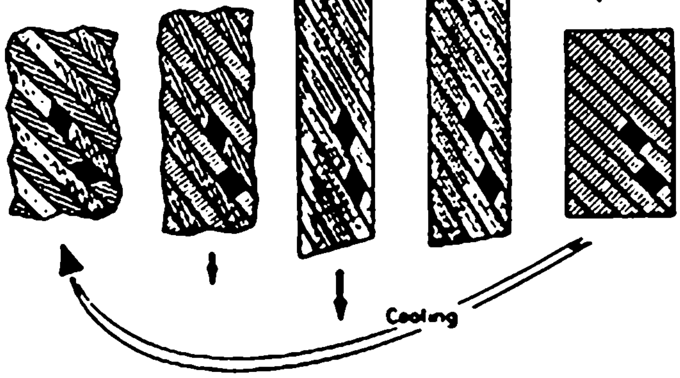

Figure 4: Model body and its deformation upon loading and heating

Statistical Mechanics

Statistical mechanics recognizes the fact that in all deformations two opposing tendencies compete: the tendency of the energy U to become minimal by pulling the body into its potential wells and the tendency of the entropy S to become maximal by letting the body occupy all positions with equal probability. In this competition it is in fact the free energy

$$F = U - TS \tag{2}$$

which becomes minimal.

In this present case the free energy has the form

$$F = \sum_{\Delta} \Phi(\Delta)\, N_{\Delta} + 2\,\frac{e}{N} \left(\sum_{\Delta_{t}} N_{\Delta}\right) \left(\sum_{\Delta_{A}} N_{\Delta}\right) - kT \ln \frac{N!}{\prod_{\Delta} N_{\Delta}!}\ . \tag{3}$$

The first term obviously denotes the potential energy of the N layers while the last term is the usual statistical expression for the entropy. The second term represents the interfacial energy between austenitic and martensitic layers. e is the energy of such an interface and the two sums over the martensitic and austenitic shear lengths are proportional to the expectation value of the number of such interfaces.

The distribution function N_{Δ} appropriate for equilibrium is calculated by minimizing the free energy under the constraint (1). Once this distribution function is known, we may calculate the free energy F as a function of deformation and temperature and, by differentiation with respect to D, the load as a function of D and T. For details of this calculation the reader is referred to [2]. The results are represented in Figure 5. Inspection shows that the

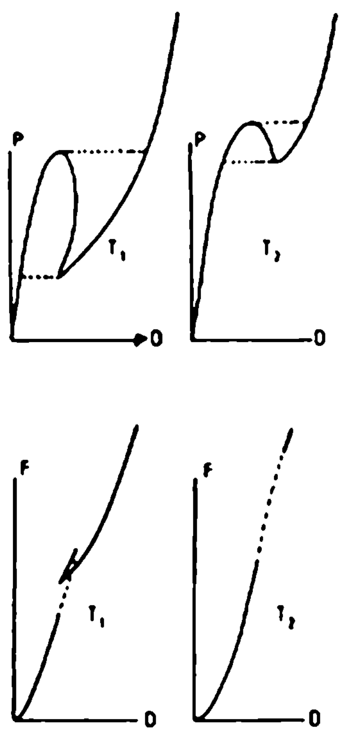

Figure 5: Non-convex free energies and non-monotone load-deformation curves

free energies are non-convex functions of D and that the load-deformation curves may imply a hysteresis in a loading-unloading experiment. Indeed upon loading, the load cannot on the left branch surpass the maximum; therefore, a break-through on the right branch will occur. Analogously, upon unloading, the break-through will occur when the load falls below the minimum. These break-through lines have been indicated in Figure 6 by the horizontal dotted lines which define the upper and lower boundaries of a hysteresis region.

Thus we conclude that the model is capable of simulating pseudoelasticity and, in particular, the pseudoelastic hysteresis.

Kinetic Theory

In order to be able to treat transient phenomena in shape memory alloys we have formulated an internal variable theory of the model which considers the phase transition and the twinning as an activated process. For the full description of that theory and its exploitation we refer the reader to [3]. Here we present an abbreviated version.

The fractions $x_{M_\pm}$ and x_A of martensitic and austenitic layers are supposed to be governed by rate laws, viz.

$$\begin{aligned} \overset{\circ}{x}_{M_-} &= -\overset{-\circ}{p}\, x_{M_-} + \overset{\circ-}{p}\, x_A \\ \overset{\circ}{x}_A &= \overset{-\circ}{p}\, x_{M_-} - \overset{\circ-}{p}\, x_A - \overset{\circ+}{p}\, x_A + \overset{+\circ}{p}\, x_{M_+} \\ \overset{\circ}{x}_{M_+} &= \overset{\circ+}{p}\, x_A - \overset{+\circ}{p}\, x_{M_+} \end{aligned} \tag{4}$$

Thus the rate x_{M_-} consists of a gain and a loss. The loss comes from the layers that jump from the left minimum to the central one and the gain is due to jumps in the opposite direction. Those jumps are governed by transition probabilities, e.g. $\overset{-\circ}{p}$ which we assume to be given by the expression

$$\overset{-\circ}{p} = \sqrt{\frac{kT}{2\pi m}}\; e^{-\frac{\Phi(\Delta_L) - P\Delta_L}{kT}}\; e^{-\frac{2\sigma(1-2x_M)}{kT}} \tag{5}$$

The first exponential factor represents the probability for a layer to have a shear length equal to the abscissa of the left maximum of the potential energy function. It must be noted here that under a load the potential energy of a layer is equal to $\Phi(\Delta) - P\Delta$, i.e., the presence of the load distorts the potential energy function $\Phi(\Delta)$ by adding the potential energy of the load which is a linear function of Δ.

The second exponential factor in equation (5) represents the probability of a change in interfacial energy. The square root in front of the exponentials is the rate with which the layers run against their barriers.

Given P(t) and T(t), two functions of time, the equations (4) may be used to calculate the phase fractions $x_{M_\pm}(t)$, $x_A(t)$ as functions of time by successive integration. Once these are known we may determine the deformation D(t) as a function of time from

$$D = \frac{1}{\sqrt{2}}\left(x_{M_-}\frac{\sum\limits_{M_-}\Delta e^{-\frac{\Phi(\Delta)-P\Delta}{kT}}}{\sum\limits_{M_-} e^{-\frac{\Phi(\Delta)-P\Delta}{kT}}} + x_A\frac{\sum\limits_{A}\Delta e^{-\frac{\Phi(\Delta)-P\Delta}{kT}}}{\sum\limits_{A} e^{-\frac{\Phi(\Delta)-P\Delta}{kT}}} + x_{M_+}\frac{\sum\limits_{M_+}\Delta e^{-\frac{\Phi(\Delta)-P\Delta}{kT}}}{\sum\limits_{M_+} e^{-\frac{\Phi(\Delta)-P\Delta}{kT}}} \right) \tag{6}$$

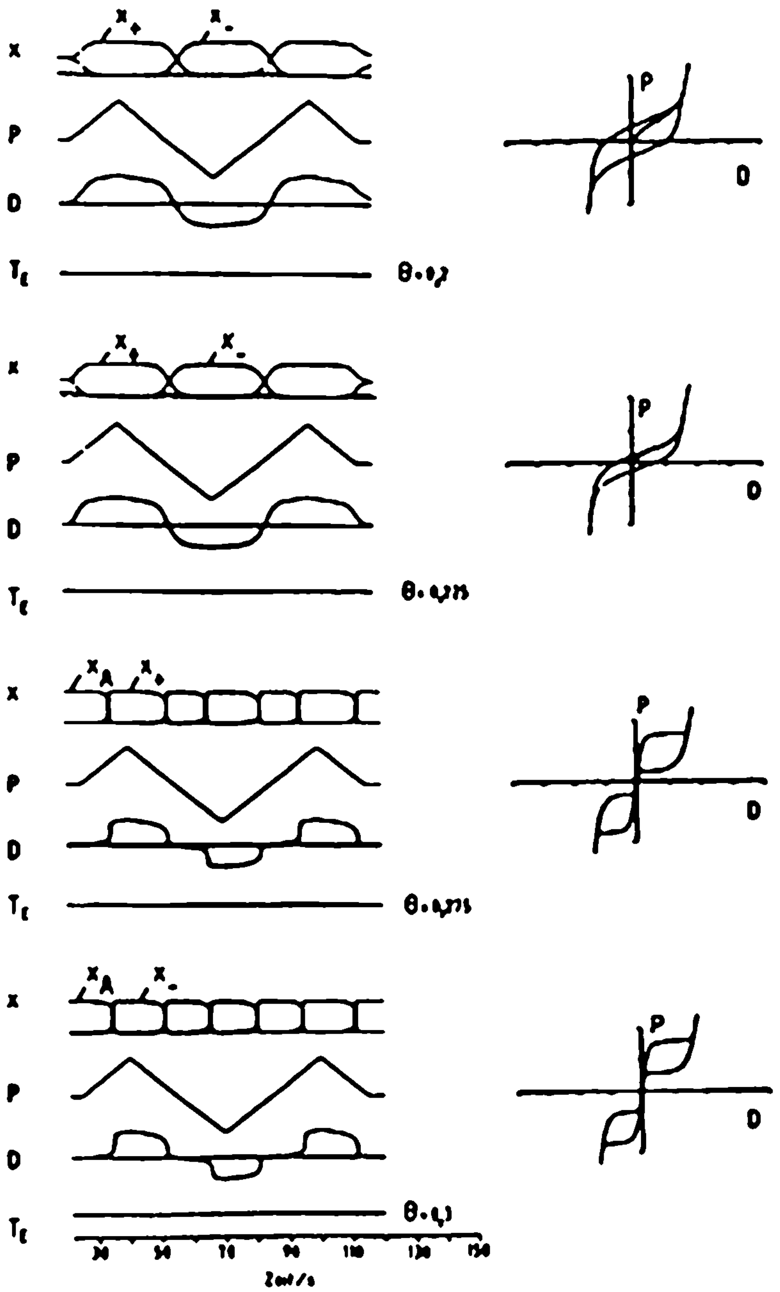

Figure 6: Phase fractions and deformations calculated as functions of time for given loads and temperatures

Figures 6 and 7 show some results. In Figure 6 the model is subject to alternating tensile and compressive forces at fixed temperatures. The phase fractions and deformations are calculated and plotted. On the right hand side we have plotted the load-deformation curves implied by these calculations. Inspection shows that these curves exhibit all the qualitative features of the schematized experimental plots of Figure 1. Figure 7 must be compared to Figure 2, because here we subject the model to a triangular tensile load and to a heating-cooling cycle. The deformation is calculated and shown in the lower diagram of Figure 7 and it shows all the qualitative features of the observed curve D(t) in Figure 2.

Thus we come to the conclusion that the kinetic theory of our model simulates the observed phenomena well.

Width of the Hysteresis

We turn back to the non-monotone load-deformation curves of Figure 6 which were derived by statistical arguments and which we have used to construct hysteresis loops.

The prototype of non-monotone load-deformation curves is provided by the van-der-Waals equation for vapours and liquids. But between vapours and liquids a hystersis is usually absent. Rather there is a horizontal line of fixed pressure on which the phase transition proceeds in both directions. In the present case that line should be constructed by bisecting the "non-monotone region" of the (P,D) - diagram as shown in Figure 8. (Maxwell's equal area rule). In the (P,D)-diagram the load of the reversible phase transition represents the slope of the common tangent to the convex parts of the free energy. The body prefers the tangent, because for a given D it provides a lower free energy than the curve P(D,T) itself.

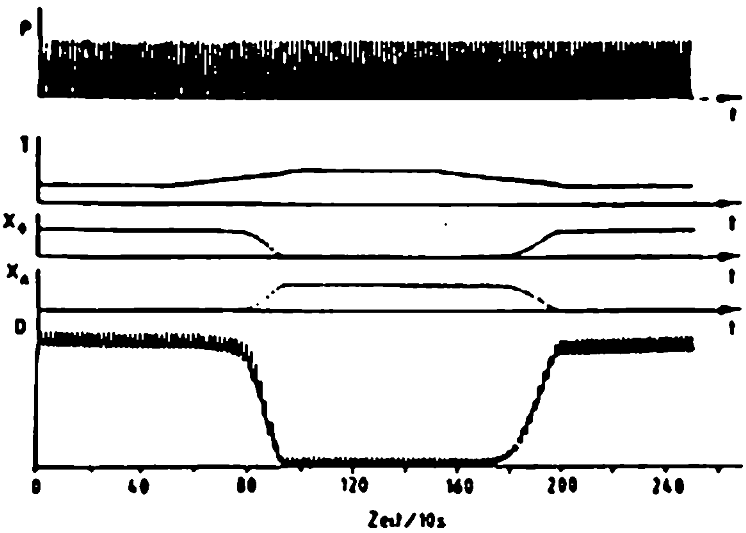

Figure 7: Model subject to a triangular tensile load and to a heating-cooling cycle.

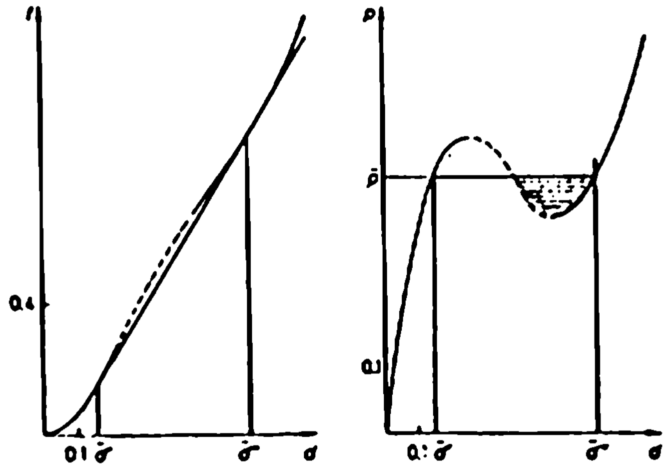

Figure 8: Maxwell construction for a reversible phase transition.

The question arises why the liquid-vapour phase transition is reversible while a phase transition in solids is invariably connected with a hysteresis. In a recent paper [4] Müller provides an answer to that question. He argues that Maxwell's argument ignores interfacial energies between austenitic and martensitic regions in the phase mixture. And he suggests an argument by which the interfacial energy may be used to relate the width of the hysteresis to the size of the interfacial energy.

References

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(4) Müller, I.: On the Size of the Hysteresis in Pseudoelasticity. Cont. Mech. and Thermodynamics 1 (1989).