

## Modeling Of Hysteresis In Martensite Transformation

L.LÜ, E.AERNOUDT AND L.DELAIEY  
 Dept. of Metall. and Mat. Eng., K.U. Leuven  
 De Croylaan 2, B-3030 Heverlee

### Introduction

The Martensitic transformation is characterized by a cooperative shear movement of atoms. Since it is a diffusionless transformation, in general there is no change in chemical composition associated with the forward and the reverse transformations. The martensitic transformation, is driven by the free energy difference between the parent phase and the martensitic phase. It may be initiated both by lowering the temperature below  $M_s$  and/or by applying a stress above  $M_s$ . A supercooling below the equilibrium temperature  $T_0$  or the application of stress is necessary to overcome several nonchemical energy terms which oppose the chemical driving force. Likewise, for the reverse transformation, a super heating above  $T_0$  or the release of a stress is required if we want the reverse transformation to take place(1). No matter how, in any case, there is a zone of temperatures  $\Delta T$  or stresses  $\Delta \sigma$ , spanning the initiation and completion of both forward and reverse transformation, which is referred as hysteresis. This hysteresis behaviour is related with the energy dissipation(2,3) and the sources of hysteresis have been discussed in detail in other papers(4,5).

In the present hysteresis model, the attention is focused on the macroscopic behaviour of shape memory alloys during the transformation. The microscopic behaviour and related phenomena are considered only indirectly. The model can simulate full and partial martensitic transformations and also predict the shifting of transformation return points during partial cooling and heating cycles.

### Thermodynamic transformation

The free energy difference between the two phases in the case of diffusionless transformation is defined as the chemical driving force. Since the free energy of a system is

$$G = -TS + pV + U \quad (1)$$

where  $G$  is the free energy,  $U$  the internal energy,  $T$  the temperature,  $S$  the entropy,  $p$  the pressure and  $V$  the volume, the free energy difference between the parent and the martensitic phase is:

$$\Delta G^{P-M} = G^M - G^P = -\Delta S^{P-M}T + p\Delta V^{P-M} + \Delta U^{P-M} \quad (2)$$

where  $\Delta S^{P-M}$  is the entropy difference between the parent phase and the martensitic phase,  $\Delta U^{P-M}$  the internal energy difference and  $\Delta V^{P-M}$  represents the volume change during transformation.

For an infinitesimal change in temperature and pressure, the change in the free energy difference is:

$$\begin{aligned} d\Delta G^{P-M} &= d\Delta U^{P-M} - \Delta S^{P-M}dT - Td\Delta S^{P-M} + \Delta V^{P-M}dp + pd\Delta V^{P-M} \\ &= -\Delta S^{P-M}dT + \Delta V^{P-M}dp \end{aligned} \quad (3)$$

Since a stress field  $\sigma_{ij}^I$  is built up due to elastic accommodation during thermoelastic transformation, the free energy in the material is altered due to that stress field. The energy change includes two parts. One of them is elastic energy which is stored in the material. Another part of energy is used for the interface motion under stress field  $\sigma_{ij}^{IF}$ . This part of energy is considered as dissipated energy. The total energy change hence reads:

$$d\Delta G_{nch}^{P-M} = dE_{el} + dE_{irr} \quad (4)$$

Following Kato(7), the stored elastic energy is:

$$dE_{el} = \sigma_{ij}^I e_{ij}^I dv / 2 \quad (5a)$$

In Eq.(5a) the superscript I represents the internal field,  $\sigma_{ij}^I$  internal stress and  $e_{ij}^I$  the elastic strain which is induced by the elastic growth of martensite during thermoelastic transformation. The irreversible energy can be written as:

$$dE_{irr} = \sigma_{ij}^{IF} e_{ij}^{IF} dv \quad (5b)$$

where  $\sigma_{ij}^{IF}$  is the average stress for the interface motion and  $e_{ij}^{IF}$  the interface motion strain.

In linear elasticity, the stress tensor  $\sigma_{ij}^I$  is related to the elastic strain tensor  $e_{ij}^I$  through Hooke's law:

$$\sigma_{ij}^I = C_{ijkl} e_{kl}^I \quad (5c)$$

The work performed under stress field  $\sigma_{ij}^I$  and  $\sigma_{ij}^{IF}$  can be represented as follows

$$d\Delta G_{nch}^{P-M} = C_{ijkl} e_{kl}^I e_{ij}^I dv/2 + \sigma_{ij}^I P e_{ij}^I dv \\ = dE_{el} + dE_{irr} \quad (6)$$

Besides the elastic energy and irreversible energy, surface energy is created with the formation of new interfaces between parent and martensite phases during transformation(6). It is

$$dE_{sur} = \Gamma dA \quad (7)$$

where  $\Gamma$  is the interface energy per mole/m<sup>2</sup> and A the area of interface. The contribution of  $E_{sur}$  to the energy balance is very small(8) and will be neglected.

In the case of the application of an external force, the free energy will change due to the elastic strain field  $e_{ij}^E$ , which gives a work term:

$$dW = V \sigma_{ij}^E d e_{ij}^E \quad (8)$$

where superscript E represents the external origin of the field and  $V$  the volume of material. As a matter of fact, this energy is different from the stored elastic energy. It promotes the forward transformation.

The free energy change during transformation is the summation of chemical energy, friction energy, elastic stored energy, surface energy and external work. It reads:

$$d\Delta G^{P-M} = d\Delta G_{ch}^{P-M} + dE_{irr} + dE_{el} + dE_{sur} + dW \\ = -\Delta S dT + \Delta V^{P-M} dp + C_{ijkl} e_{kl}^I e_{ij}^I dv/2 \\ + \sigma_{ij}^I P e_{ij}^I dv - V \sigma_{ij}^E d e_{ij}^E \quad (9)$$

In every local equilibrium, the free energy change should satisfy the equilibrium condition:

$$0 = d\Delta G_{ch}^{P-M} + dE_{irr} + dE_{el} + dW \quad (10)$$

In the Eq.(10)  $d\Delta G_{ch}^{P-M}$  is due to the free energy difference between two phases,  $dE_{irr}$  represents all the dissipated energy (mainly friction energy of interface motion),  $dE_{el}$  is the stored elastic energy during the nucleation and growth of martensitic plates during the forward transformation and the term  $dW$  is the increment of energy relied on the application of external force.

## Modeling of transformation

### 1. Stored Elastic Energy

To illustrate the model, we start the discussion with a special case: a bar which is trained as a shape memory operator (SMO) has the stress-strain relation shown in Fig.1. We also assume that

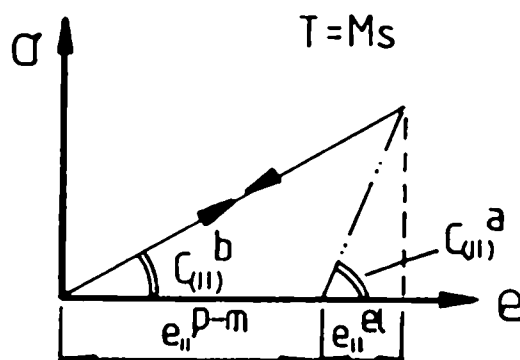


Fig.1. Schematic representation of mechanical behaviour of SMO.

the energy dissipation during the forward and the reverse transformation approaches zero. At a constant temperature  $M_s$ , the stress control parameter is applied to the SMO. Since there is no energy dissipation, equation (10) is simplified to:

$$0 = d\Delta G_{ch}^{P-M} + dE_{el} + dW$$

$$= -\Delta SdT|_{M_s} + C_{ijkl} e_{kl}^I e_{ij}^I dv/2 - V_0 \sigma_{11}^E de_{11}^E \quad (11a)$$

where  $\sigma_{11}^E$  and  $e_{11}^E$  respectively represent the stress and the macroscopic deformation of the SMO. All the energy due to cooling from  $T_0$  to  $M_s$  and due to the application of external work is stored as elastic energy in the operator because of no energy dissipation. So in the case of uniaxial tensile loading the internally stored elastic energy should satisfy

$$dE_{el} = C_{ijkl} e_{kl}^I e_{ij}^I dv/2$$

$$= SdT|_{M_s} + V_0 \sigma_{11}^E de_{11}^E$$

$$= SdT|_{M_s} + V_0 \sigma_{11} (de_{11}^{P-M} + de_{11}^{el}) \quad (11b)$$

since the total strain includes two parts: 1). transformation strain  $e_{11}^{P-M}$  and 2). elastic strain  $e_{11}^{el}$  caused by applied tensile stress.

According to Fig.1

$$C_{1111}^b (e_{11}^{P-M} + e_{11}^{el}) = C_{1111}^a e_{11}^{el} \quad (12a)$$

where  $C_{1111}^a$  is the modulus of parent phase and of the martensite phase (for a convenience assumed to be equal to each other) and  $C_{1111}^b$  the transformation modulus

$$e_{11}^{el} \left(1 - \frac{C_{1111}^b}{C_{1111}^a}\right) = \frac{C_{1111}^b}{C_{1111}^a} e_{11}^{P-M} \quad (12b)$$

Let  $\frac{C_{1111}^b}{C_{1111}^a} = p$

and we get

$$e_{11}^{el} = \frac{p}{1-p} e_{11}^{P-M} \quad (12c)$$

$$de_{11}^{el} = \frac{p}{1-p} de_{11}^{P-M} \quad (12d)$$

Substituting  $e_{11}^{el}$  and  $de_{11}^{el}$  into Eq.(11b), we can obtain the stored energy change as a function of forward transformation strain  $e_{11}^{P-M}$ :

$$dE_{e1} = \Delta SdT|_{Ms} + C_{1111}^b \left(\frac{1}{1-p}\right)^2 v_0 e_{11}^{P-M} de_{11}^{P-M} \quad (13a)$$

Let  $C_{1111}^b \left(\frac{1}{1-p}\right)^2 v_0 = A$  so that

$$dE_{e1} = \Delta SdT|_{Ms} + A e_{11}^{P-M} de_{11}^{P-M} \quad (13b)$$

Clearly, Eq.(13b) means that the stored energy due to nucleation, growth of martensitic plates etc is a parabolic function of transformation strain. This result is in agreement with the experimental data obtained by Planes et al(10). Here we only consider the total stored energy since all the stored energy due to transformation has the same action which is to oppose forward transformation, and to help the reverse transformation. Replacing  $dE_{e1}$  in Eq.(10) with Eq.(13b), we obtain

$$0 = -\Delta SdT + \Delta v^{P-M} dp + (\Delta SdT|_{Ms} + A e_{11}^{P-M} de_{11}^{P-M}) + \sigma_{ij}^I \epsilon_{ij}^F dv - v_0 \sigma_{ij}^E de_{ij}^E \quad (14a)$$

For the reverse transformation we just rewrite Eq.(14a) as

$$0 = -\Delta SdT + \Delta v^{M-P} dp + (\Delta SdT|_{Ms} + A e_{11}^{M-P} de_{11}^{M-P}) - \sigma_{ij}^I \epsilon_{ij}^F dv - v_0 \sigma_{ij}^E de_{ij}^E \quad (14b)$$

## 2. Dissipated Energy

For the simplification, we assume that the energy dissipation is a linear function of the transformation strain  $e_{11}$ . Therefore the forward transformation:

$$dE_{irr} = \mu de_{11}^{P-M} \quad (15a)$$

where  $\mu$  is a proportional constant. For the reverse transformation, we assume that the dissipated energy is reset to zero because there is no energy dissipation at the beginning of the reverse transformation. The energy dissipation also increases linearly with the amount of reverse transformation strain:

$$dE_{irr} = \mu d(e_{11}^{P-M}[\text{return}] - e_{11}^{M-P}) \quad (15b)$$

where  $e_{11}^{P-M}[\text{return}]$  is the SMO strain in which forward transformation returns and  $e_{11}^{M-P}$  the SMO strain on reverse transformation.

### Simulation of hysteresis

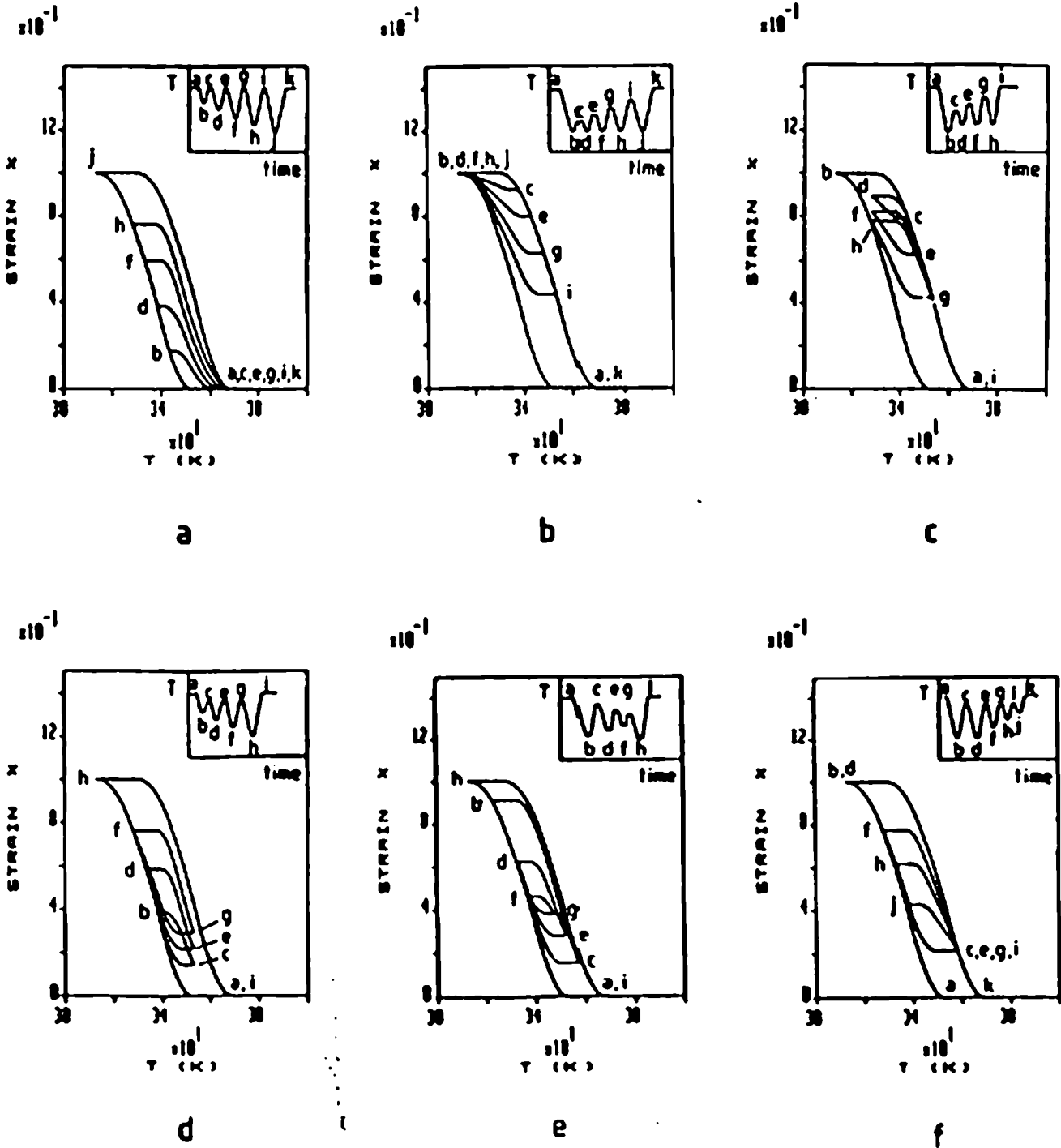
In order to simulate hysteresis of a specimen during martensitic transformation, we assume that:

1. The specimen consists of multiple SMO's which are parallelly linked together;
2. Every SMO has different equilibrium temperatures  $T_0^*$  and  $M_s^*$ ;
3. There is no interaction among the SMO and
4. The deformation of the specimen is the total contribution of every SMO and the deformation of the specimen obeys the relation as following:

$$e_s = \frac{1}{n} \sum_{i=1}^n e_i \quad (16)$$

where  $e_s$  is specimen strain and  $e_i$  the strain of SMO  $i$  when it would be disconnected from the other SMO. Summation is from the first SMO until the last SMO.

Fig.2a to 2f show a set of simulated hysteresis loops where the parameters are chosen as  $C_{1111}^a = 50000$  MPa,  $C_{1111}^b = 10000$  MPa, entropy difference between two phases  $S = 3$  J/mol.K, and  $\mu = 600$ . In the upper right corner of every figure, the saw-tooth profile represents the cooling-heating procedure.



**Fig.2a to 2f.** A set simulated hysteresis loops and subloops which predict special phenomena during partial forward and reverse transformation.

## Discussion

Fig.2a to 2f simulate different procedures of thermal cycling. Fig.2a and 2b show the partial cooling-full heating and full heating-partial cooling profiles. Fig.2c and 2d. represent partial transformation subloops during cooling and heating, which predict the shift of transformation return points during partial transformation although the temperatures at partial forward transformation return points(Fig.2c) or temperatures at partial reverse transformation return points(Fig.2d) are the same. Fig.2e shows that if the subsequent partial cycle loop is enveloped by previous loops (the end cooling temperature for the subsequent cycle is higher than the previous end cooling temperature and the partial heating return temperature for the subsequent cycle is lower than the previous one), the full heating path remembers all the previous return points. In Fig.2f all the partial cooling paths follow a common route c-d and they also have the same partial reverse transformation return points at a temperature of 358K (points c,f and h). Those simulated results are very well in agreement with experimental observations(10).

## Acknowledgment

The authors wish to thank Dr.J.Van Humbeeck, Dr.P.Wollants, Dr.J.Ortin, Dr.G.Gautam, M.De Graef, R.Stalmans, L.Cooreman and Y.Van der Veken for helpful discussions. Li Lü wishes to acknowledge the Department. of Metallurgy and Materials Engineering, K.U.Leuven for the financial support.

## References

- (1). K.Mukherjee, ICOMAT-2, 6-7, Aug. 1982, Leuven, Belgium,p4\_5.
- (2). R.J.Salzbrenner and M.Cohen, Acta Met. vol. 27, (1979),p739.
- (3). G.B.Olson and M.Cohen, Scripta Met., Vol. 9, (1975), p1247.
- (4). Delaey and E.Aernoudt, Proc. Inter. Confer. On Martensite ICOMAT-86, 926-933, Nara, Japan, August, 1986.
- (5). L.Delaey, J.Ortin and J.Van Humbeeck, Proc. of Phase Transformation'87, 6-10, July, 1987, Cambridge.
- (6). C.M.Wayman, Proc. 1st. JIM Inter. Sympo. On New Aspect Of Martensite Transformation, Kobe, May 10-12, (1986), p159.
- (7). M.Kato and H.R.Pak, phys. stat. sol. (b), 123, (1984), p415.
- (8). G.B.Olson and M.Cohen, Scripta Met. Vol.11, (1977), p157.
- (9). A.Planes, J.L.Maequeeron and J.Ortin, Phil. Mag. Lett. Vol.57, (1988), p291.
- (10).Lü Li, ph.D thesis, in progress.