Orissa Journal of Physics © Orissa Physical Society Vol. 19, No.1
ISSN 0974-8202 February 2012
pp. 49-56

Utilization of Mathematical Model to Understand Martensitic Transformation in Ferromagnetic Shape Memory Alloys

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Received : 12.12.2011 ; *Accepted* : 6.01.2012

Abstracts: Ferromagnetic Shape Memory Alloys (FSMAs) are the highly demanding material for engineering application. It has the ability to return to a predetermined shape by application of thermal field or magnetic field. The key characteristic of Shape Memory Alloys are the occurrence of a martensitic phase transformation which is a phase change between two solid phases and involves rearrangement of atoms within the crystal lattice. In this article, the basic phenomena and concepts of martensitic transformation along phase changes in FSMAs are presented through mathematical models. The implementation of mathematical calculations of FSMAs in to engineering applications are impeded by the absence of a theory that would allow to complete the thermo-mechanical characteristics of polycrystalline and can be effectively adapted to the analysis of SMAs dynamics as well as to other problems on structural phase transition. Shape recovery by thermal and magnetic field and the role of twin boundary symmetry are briefly reviewed. This paper formulates the initial and boundary conditions for evaluation of result of the system are considered.

Keywords: Ferromagnetic Shape Memory Alloys; Transformation Temperature; Shape Memory Effect.

1. Introduction

Shape-memory technologies are now-a-days exploited in a variety of different applicative contexts ranging from sensors and actuators (even microscopical) [1-2], to robotics [3], to clamping and fixation devices [4], to space applications (grippers, positioners) [5], to damping devices (shock absorption) [6], to biomedical applications [7, 8]. When a Shape Memory Alloy is cold, or below its transformation temperature, it has a very low yield strength and can be deformed quite easily into any new shape, which it will retain. However, when the material is heated above its transformation temperature it undergoes a change in crystal structure which causes it to return to its original shape [9-12]. The shape memory effect can be described to a phase transition between two different configurations of the metallic lattice (martensite and austenite). The martensitic transformation is associated with an inelastic deformation of the crystal lattice with no diffusive process involved. The phase transformation results from a cooperative and collective motion of atoms on distances smaller than the lattice parameters. Martensite plates can grow at speeds which approach that of sound in the metal (up to 1100m/s). Together with fact, that martensitic transformation can occur at low temperatures where atomic mobility may be very small, results in the absence of diffusion in the martensitic transformation within the time scale of transformation. The absence of diffusion makes the martensitic phase transformation almost instantaneous (a first-order transition). When a shape memory alloy undergoes a solid-to-solid phase transformations, it transforms from its high symmetry austenite phase (typically cubic) to a low symmetry several martensitic phase (i.e. tetragonal, trigonal, orthorhombic or monoclinic) which occur in various variants (mostly 3, 4, 6 or 12) [13]. The transformation phenomenon diagrammatically represents in figure-1, in which M_s, M_f, A_s and A_f are denoted as martensitic starting temperature, martensitic finish temperature, austenitic starting temperature and austenitic finish temperature respectivelly; In the absence of stress.

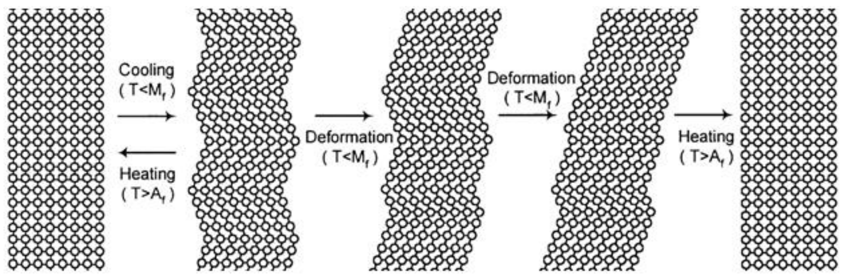


Fig. 1: Graphical Mechanism of shape recovery of SMAs

Many mathematical models are derived to relate with the effects of SMAs [14-18]. Here FSMA phenomenons are described to better understanding about phase transformation, twin boundary movement, etc.

2. Thermal shape memory effect

Let the fraction of martensite present in the material is f_m at a temperature T, during the phase transformation in FSMAs. The model condition represents the material contains some martensite M_{fo} and some austenite (1- M_{fo}) at a temperature T_0 (as shown infigure-2).

2.1 For austenite to martensite transformation

As in the figure-2, we can describe the behavior of the plot as the cosine function i.e.

$$f_m = A\cos\theta + B = A\cos\alpha_m (T - M_f) + B \tag{1}$$

The boundary condition will be,

$$f_m = 0 \text{ at } \theta = \pi, \quad \text{So, } A = B$$

and $$f_m = 1 \text{ at } \theta = 0, \quad \text{So, } A = B = \frac{1}{2}$$

So, the mathmetical expression based on either the material being in fully martensitic or fully austenitic phase at initial stage of transformation. At martensitic starting temperature (M_m), the material is in austenitic phase. So $f_m = 0$ and $\theta = \pi$. So we can write from equation-1;

$$0 = A\cos\alpha_m (M_s - M_f) + B$$

So $$\alpha_m = \frac{\pi}{M_s - M_f} \quad (\text{for } M_f \le T \le M_s) \tag{2}$$

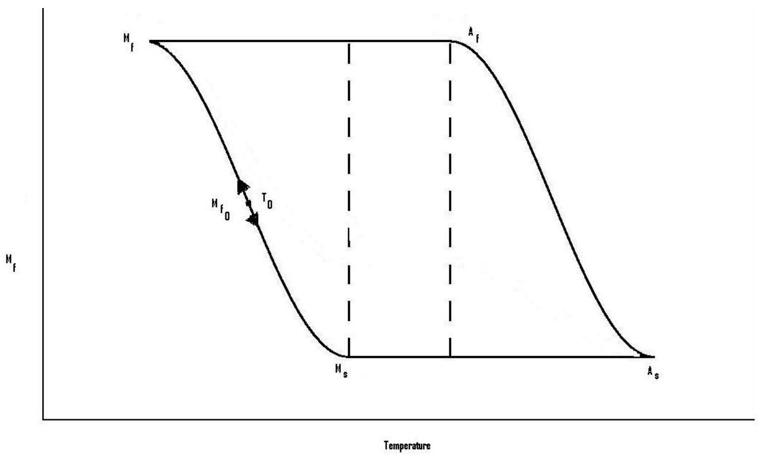


Fig. 2: Thermo elastic - martensitic transformation.

2.2 For martensite to austenite transformation

From equation-1, the transformation can be written as,

$$f_m = \frac{1}{2}\cos\alpha_A (T - A_s) + \frac{1}{2}$$

So, $$\alpha_A = \frac{\pi}{A_f - A_s} \quad (\textit{for } A_s \le T \le A_f) \tag{3}$$

The above mathematical expressions (2) & (3) can be modified as based on; no new martensite is added until the temperature T_0 reaches to M_s. Consider the process would start at some value Mf_0 at temperature T_0 .Concerning the two phases, coexistent of martensite and austenite are considered at each point.

The boundary condition will be,

$$f\,m = fm_0 \;\text{ at }\; \theta = \pi$$

and $\quad f\,m = 1 \;\text{ at }\; \theta = 0$

Hence, $\quad A = \dfrac{1 - fm_0}{2} \quad$ and $\quad B = \dfrac{1 + fm_0}{2}$

So, equation (1) can be written as,

$$f_m = \frac{1 - fm_0}{2}\cos(\alpha_m (T - M_f)) + \frac{1 + fm_0}{2} \tag{4}$$

For martensite to austente with $f_m = fm_o$ & $T = T_0$ on the basis that no new austenite is formed until the temperature reaches A_s.

The boundary condition will be,

$$fm = fm_0 \;\text{ at }\; \theta = 0$$

and $\quad fm = 0 \;\text{ at }\; \theta = \pi$

Hence, $\quad A = B = \dfrac{fm_0}{2}$

So, $\quad f_m = \dfrac{fm_0}{2}\cos(\alpha_A (T - A_s)) + 1 \qquad (5)$

3. Magnetic Shape Memory Effect

The essential condition for this model is the driving force of twin boundary motion i.e. rearrangement of the martensite microstructure which is the difference in magnetization free energy between different martensitic variants.

But the magnetic anisotropy of the alloy is a crucial parameter and that driving force cannot exceed its saturation value [19].

Let the driving force (i.e. magnetic stress) is σ_m.

$$f\,m = fm_0 \;\text{ at }\; \theta = \pi$$

and $\quad f\,m = 1 \;\text{ at }\; \theta = 0$

Hence, $\quad \alpha_m = \left(\int_0^H M_{001}(H)\,dH - \int_0^H M_{100}(H)\,dH \right) \dfrac{1}{10} \qquad (6)$

where H= the strength of magnetic field, M_{001} & M_{100} are magnetization of the martensitic variants with [001] & [100] directions along the magnetic field. $\varepsilon_0 = \left(1 - \frac{c}{a}\right)$ is the distoration of the lattice.

When the external stress σ_{EXT} is considered, the model gives a net driving stress;

$$\sigma_m(H) - \sigma_{EXT}$$

Hence, the twin boundaries move as far as the condition satisfied. The condition is;

$$\sigma_m(H) - \sigma_{EXT} > \sigma_{TW}(\varepsilon) \tag{7}$$

Based on this relation a macroscopic strain dependency ε(H) can easily determined. The $\sigma_{TW}(\varepsilon)$ dependence and magnetization curves as well as the distortion of the lattice can be obtained experimentally.

The maximum possible driving force can be determined from equation-6 as,

$$\sigma_m^{\max} = \frac{k1}{z0} \tag{8}$$

where $K1$ is uniaxial anisotropy constant of the martensite.

Hence the existence of magnetic shape memory effect can be predicted by combining equation-6 and -8;

$$\frac{K1}{z0} > \sigma_{TW} + \sigma_{EXT} \tag{9}$$

By taking arbitrary macroscopic strain $\varepsilon < \varepsilon_0$,

$$\frac{K1}{z0} > \sigma_{TW}(\varepsilon) + \sigma_{EXT} \tag{10}$$

Hence, the equation-10 can predict the possibility of observing the threshold macroscopic strain.

For reversible magnetic shape memory effect, it follows that the two separate reorientations mentioned above can be combined into a single experiment with constant external stress, provided that the condition is fulfilled i.e.

$$\frac{K1}{z0} > \sigma_{TW} > +\sigma_{EXT} \tag{11}$$

The condition will be possible for the specimen with

$$\frac{K1}{z0} > 2\sigma_{TW}$$

The relationship-11 states that the maximum magnetic stress $\left(\frac{k1}{\varepsilon 0}\right)$ must overcome the sum of twining stress and external stress which facilitates the [001] => [100] reorientation along the constant external stress when the magnetic field reaches a larger enough magnitude. And it can be states that at the same time the constant external stress must be higher than the twinning stress which facilitate the reverse reorientation, [100] => [001] along the external stress, when the magnetic stress decreases below certain level.

4. Twin boundary orientation in Ni-Mn-Sn FSMA

It is known that Ni-Mn-Sn FSMAs is a ternary intermetallic compound, which has the cubic $L_2$1-type structure in its parent phase. In this structure, the Ni ion occupy at the site of the cube corners (8c-site), and Mn and Sn ions are in the alternate body centers of the successive cubes (4a- and 4c- sit, respectively) [20], as shown in figure-3. During transformation, (100) orientation of the orthorhombic unit cell as derived from a (100) orientation of the cubic unit cell can be depicted by a 2-dimensional projection shown in Figure-4.

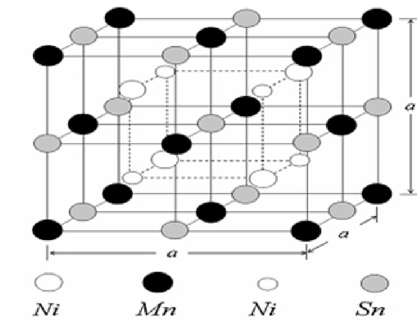
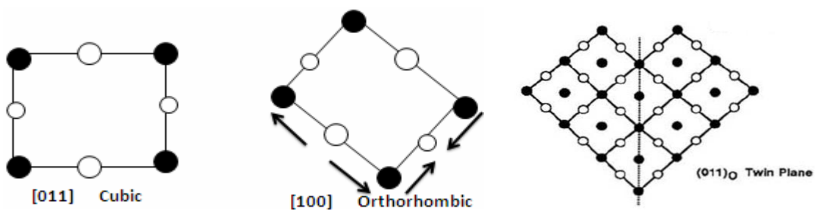


Fig. 3: Different atomic sites are presented in Unit cell of Ni-Mn-Sn FSMA.



(a) (b) (c)

Fig. 4: Structural representation (a) for cubic with [011], (b) for orthorhombic with [100] and (c) for twin boundary orientation in between them with (011) plane.

Twinning on the (011) plane, which is not a plane of symmetry [21]. Using the lattice parameters listed above for the orthorhombic unit cell, the distortion matrix can write with respect to the orthorhombic axes as;

$$T = \begin{bmatrix} \frac{c}{\sqrt{2a0}} & 0 & 0 \\ 0 & \frac{c}{\sqrt{2a0}} & 0 \\ 0 & 0 & \frac{c}{\sqrt{2a0}} \end{bmatrix}$$

With the rotation matrix between me twins as: $T = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$, where

$\phi = 3.24^{o}$.

6. Conclusion

Good agreement of the presented experimental and the theoretical model supports its validity and demonstrates that this model can be suitable for describing the phenomenological aspects of magnetic shape memory effect (MSME) such as temperature limits, reversible behavior and magnetic field induced superelasticity.

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