Analytical Description of Pseudo-Plasticity

Andrew Rusinko

Óbuda University, Népszínház u. 8, H-1081 Budapest, Hungary
ruszinko.endre@bgk.uni-obuda.hu

Abstract: As phase transformations are finding ever-widening applications, the problem of their modeling upon the application of thermal and/or mechanical loadings arises. This has resulted in a number of analytical models to describe the phenomena resulted from the phase transformation. This paper is aimed at presenting the model of PT-induced deformation in terms of the synthetic theory. After the basic, general equations are developed, the case of pseudo-elasticity will be considered in more detail.

Keywords: Phase transformation (PT), PT-induced deformation, effective temperature, pseudo-elasticity, synthetic theory

1   Introduction

Let us start with the definition of phase transition (PT). There exists a temperature-diapason within which materials undergo so-called phase transformations. PTs do not occur by the long-range diffusion of atoms but rather by some form of cooperative, homogeneous movement of many atoms that results in a change in crystal structure. These movements are small, usually less than interatomic distances, and the atoms maintain their relative arrangemets. The PT temperature interval is different for different metals and alloys. For example, iron has body-centered cubic structure (BCC) at temperature below 910°C, face centered cubic structure (FCC) for the temperature range from 910°C to 1391°C; iron structure above 1392°C returns to BCC structure. The phase transformation in tin starts at the temperature of 18°C; titanium, whose melt point is of 1660°C, has hexagonal close packed (HPC) structure below 882°C and BCC structure at higher temperature. Following [1], a low-temperature phase is called martensite or martensitic phase and a high-temperature phase − austenite or austenitic phase. Austenite→martensite transformation is referred to as direct transformation and martensite→austenite transformation is called the reverse transformation.

Phase transformations of most metals are not accompanied by noticeable deformation. However, there exist such alloys whose phase transformations are

accompanied by significant non-elastic deformation. So-called Shape Memory Alloys (SMAs) belong to them. The shape memory alloy (also known as a smart alloy, memory metal, or muscle wire) is an alloy that "remembers" its shape, and can be returned to that shape after being deformed, by applying heat to the alloy. A typical representative of SMA is nickel-titanium (Ni-Ti) alloy (metallide with approximately equal Ni- and Ti-concentrations). In temperature interval from -150 to +200°C, this alloy undergoes phase transformations, the character and sequence of which depends on the component-concentration and experimental details. In nickel-titanium alloy Ni-Ti (~45% Ni) only martensite→austenite transition upon heating and austenite→martensite transition upon cooling occur, whereas Ni-Ti 55 at.% Ni alloys undergoes so-called two-step phase transformations, upon heating, the martensitic phase first transforms into an intermediate structure and then the austenitic phase starts to grow. There is a situation such that a heat-induced intermediate phase does not nucleate, whereas it arises upon cooling.

Another important feature of martensite/austenite transformations is their reversibility. This means that the kinetics of atoms and their rearrangements in direct and reverse transitions are identical. Further, during both cooling and heating, PT can be terminated at any stage and redirected in the opposite direction. In constant temperature, the structure of load-free material remains unchangeable and there is a balance between the martensite/austenite phase and parent matrix.

2   Pseudo-Elasticity and Shape Memory Alloys

Consider the deformation of specimen loaded in tension at the temperature close to the martensite start temperature; its stress-strain diagram is shown schematically in Fig. 1. The initial portion of the diagram, segment OM_1, obeys Hooke's law. Beyond point M_1, the specimen experiences intensive flow (portion M_1M_2) caused by the formation of martensite. After the transformation is completed, beginning from point M_2, the material deforms elastically again until the yield limit σ_S is achieved (point M_3); the further increase in stress induces an usual plastic deformation. The unloading from the point lying on the portion M_1M_2 leads to the complete or partial, so-called pseudo-elastic, recover of deformation accompanied, as a rule, with a significant hysteresis. Since an unloading is equivalent to the (effective)temperature increase, the martensitic phase, which has arisen at tensile, transforms into austenitic phase. It is this fact that explains the reduction of phase-induced strain in unloading. The phase-induced strain in loading is referred to as pseudo-elasticity, which is represented by the portion M_1M_2 in Fig. 1.
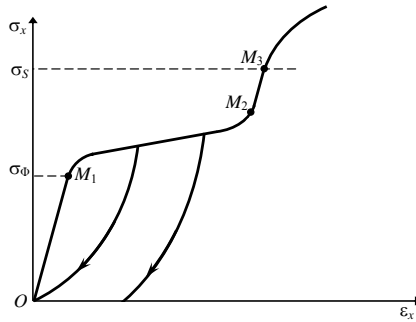
Figure 1.   Stress-strain diagram showing pseudo-elastic deformation (section M_1M_2); pseudo-elastic deformation starts arising at stress σ_Φ

Shape memory effect. Let a specimen be heated/cooled to such a temperature so that two phases are present. Further, the specimen is subjected to (a) loading in tension, (b) unloading, and (c) heating in the unloaded state. The stress-strain and strain-temperature diagram of the specimen is shown in Fig. 2. Segment OM_1 gives a pure elastic strain of the specimen. Along the portion M_1M_2, PT-induced strain is occurred, pseudo-elasticity; by the PT the martensitic transformation is meant. The portion of the diagram $OM_1M_2M_4$ in Fig. 2 is identical to the diagram in Fig. 1. After the complete unloading (point M_4) and heating (along portion M_4M_5 the strain remains unaltered), the intensive decrease in strain (portion M_5M_6) occurs that is caused by austenitic transformation due to the temperature increase.
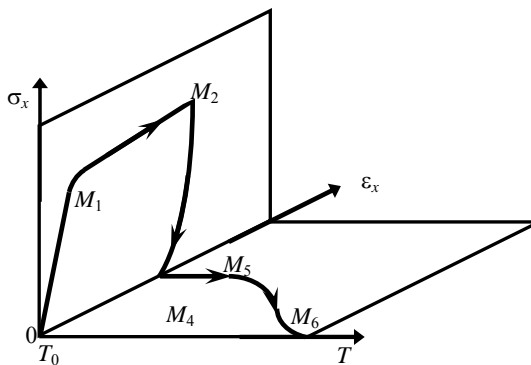

Figure 2.   Strain-strain diagram in tension showing pseudo-elastic deformation (M_1M_2) and effect of the shape memory (M_5M_6)

3   The Modeling of PT-induced Strains in Terms of the Synthetic Theory

The V.A. Lichachev and V.G. Malinin monograph [1] should be emphasized due to some principal statements are taken from it to develop the model of phase transformation induced deformation in terms of the synthetic theory.

Let a direct (martensitic, dashed arrows) or reverse (austenitic, solid arrows) transformation occurs in a local volume of body (grain); The plot of the phase character function Φ is shown in Fig. 3. The martensite formation rate is determined as

$$\dot{\Phi} = -\dot{T}*\big/\!\left(M_s - M_f{}'\right), \tag{1}$$

where $T*$ is effective temperature [1]:

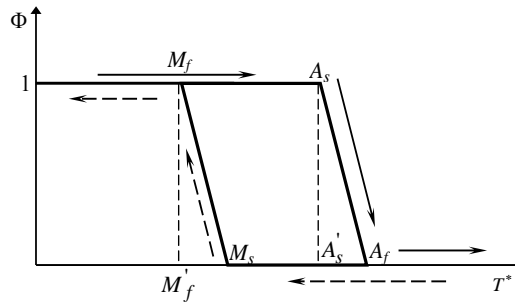$$T* = T\left(1 - D_{ij}\sigma_{ij}/q\right). \tag{2}$$

Figure 3.   Phase character function (Φ) vs effective temperature

D_{ij} are the crystal deformation components related to crystallographic axes for a complete phase transformation when the function Φ changes from zero to unit; σ_{ij} are stress components in the local volume related to the crystallographic axes; q is the phase transformation thermal effect. The components D_{ij} and q are the known physical characteristics of phase transformation for a given alloy. The martensite is formed at the reduction of $T*$ for the temperature range $M_f{}' \le T* \le M_s$. Therefore, Eq. (1) holds at $\dot{T}* < 0$ as $M_f{}' < T* < M_s$. The decrease in the martensite fraction, occurring at the effective-temperature- range $A_s{}' < T* < A_f$, is

$$\dot{\Phi} = -\dot{T}*\big/\!\left(A_f - A_s{}'\right), \tag{3}$$

i.e. Eq. (3) is applicable at $\dot{T}* > 0$ for $A_s' \le \dot{T}* \le A_f$. As $M_s - M_f{}' = A_f - A_s{}'$, Eqs. (1) and (3) are identical.

The effective temperature (2) depends on stress components acting in the local volume. As well as in the concept of slip, we assume that the state of stress in a local volume is identical to the macro-state of stress. Therefore, the components σ_{ij} in Eq. (2) are known values for a given macro-stress and, consequently, the effective temperature $T*$ is known as well. In addition, the martensite fraction can be calculated by Eq. (1) due to the temperatures M_s and $M_f{}'$ are known physical constants of material.

Now we proceed to the determination of PT-induced strain components generated in the local volume, ε_{ij}^{Φ}. In most cases, it is possible to expresses the $\dot{\varepsilon}_{ij}^{\Phi}$ components through the PT-induced lattice distortion D_{ij} and martensitic transformation rate $\dot{\Phi}$ as [1]:

$$\dot{\varepsilon}_{ij}^{\Phi} = A_{\Phi} D_{ij} \dot{\Phi}, \tag{4}$$

where A_{Φ} is the factor that takes into account that the PT-induced deformation may not be the same as the deformation of crystal lattice. However, $A_{\Phi} = 1$ is often the case. If the deformation of crystal grain is characterized by the tensor D_{ij} at the complete transformation, the average deformation of the grain at partial transformation is determined by $D_{ij}\Phi$. It is this statement that forms the basis of Eq. (4) giving $\dot{\varepsilon}_{ij}^{\Phi}$ components both at direct $(\dot{\Phi} > 0)$ and reverse $(\dot{\Phi} < 0)$ transformation.

We take Eq. (4) as the basic relationship for the determination of PT-induced strain rate components (further throughout, we will also use the phase deformation notion). To calculate by Eq. (1) the value of $\dot{\Phi}$, we need to differentiate Eq. (2) with respect to time. As a result, Eq. (4) yields the form

$$\dot{\varepsilon}_{ij}^{\Phi} = -\frac{A_{\Phi} D_{ij}}{M_s - M_f{}'}\left[\dot{T}\left(1 - \frac{D_{kl}\sigma_{kl}}{q}\right) - T\frac{D_{kl}\dot{\sigma}_{kl}}{q}\right] \tag{5}$$

In contrast to plastic deformation, the phase deformation is realized not by shears. At the same time, in most cases it is not accompanied by volume change. On the other hand, as well known, a deformation of any kind can be obtained as shears

(slips) along several (maximum 5) slip systems. This reasoning allows us to use the *synthetic theory* for the modeling of phase deformations.

In terms of the synthetic theory [2,3], each slip system is represented by tangent plane with normal vector $\vec{\mathbf{N}}$ in the Ilyushin five-dimension space and stresses σ_{kl} is replaced by scalar product $\vec{\mathbf{S}} \cdot \vec{\mathbf{N}}$, where $\vec{\mathbf{S}}$ is the stress vector. We designate through $\vec{\mathbf{e}}_0^{\Phi}$ the irreversible (phase) strain vector giving the PT-strain developed within one slip system, $\vec{\mathbf{e}}_0^{\Phi}$ is co-directed with the plane normal vector $\vec{\mathbf{N}}$. We propose to determine $\dot{\vec{\mathbf{e}}}_0^{\Phi}$, which is assumed to be co-directed with $\vec{\mathbf{N}}$ as well. Therefore, in terms of synthetic theory, Eq. (5) can be written as

$$\dot{\vec{\mathbf{e}}}_0^{\Phi} = \dot{\varphi}_N \vec{\mathbf{N}} \qquad r\dot{\varphi}_N = -\dot{T}\left(1 - D_1 \vec{\mathbf{S}} \cdot \vec{\mathbf{N}}\right) + D_1 T \dot{\vec{\mathbf{S}}} \cdot \vec{\mathbf{N}} , \qquad (6)$$

$$r = \left(M_s - M_f{}'\right)\big/\left(A_{\Phi} D\right), \quad D_1 = D/q , \qquad (7)$$

where $\dot{\varphi}_N$ is termed as strain intensity rate and D is called reduced shear for a complete transformation as the function Φ changes from 0 to 1. The reduced shear is considered as the known physical characteristic of alloy which accounts for the response of crystal grid to the phase transformation. Although the magnitude of the deformation $\vec{\mathbf{e}}_0^{\Phi}$ is a finite quantity relative to the grain size, its contribution into macro-deformation is infinitesimal due to the number of tangent planes (slip systems) is suggested to be infinite large.

The micro phase-deformation rate increment components $d\dot{e}_i^{\Phi}$ ($i = 1,2,3$) are [2,3]

$$d\dot{e}_i^{\Phi} = \left(e_0^{\Phi}\right)_i dV = \dot{\varphi}_N m_i \cos\lambda \, dV , \ \ dV = \cos\beta \, d\alpha \, d\beta \, d\lambda . \qquad (8)$$

At a point of body, the macrodeformation rate components generated in phase transformation are [2,3]

$$\dot{e}_i^{\Phi} = \iint\limits_{\alpha\ \beta\ \lambda}\!\!\int \dot{\varphi}_N m_i \cos\lambda \cos\beta \, d\alpha \, d\beta \, d\lambda , \qquad (9)$$

where $\dot{\varphi}_N$ is given by Eq. (6).

Since Eqs. (6) and (9), are obtained via Eqs. (1-3), they capable of modeling phenomena when (i) martensitic transformation induces deformation co-directed with acting stresses (ii), austenitic transformation gives the recovery of deformation.

Upon the application of both thermal and mechanical loadings, local volumes (grains) of the specimen undergo deformations induced by phase-transformations of different intensity; within some of them the phase reactions does not occur at all. In terms of the synthetic model, the local volume of body is represented by tangent plane with normal vector $\vec{\mathbf{N}}$. Therefore, first of all, it is necessary to formulate the general rule that determines the orientations of $\vec{\mathbf{N}}$ in which phase micro-deformations proceed at a given instant. The reduction of effective temperature T^* in the range $M_f' < T^* < M_s$ (Fig. 3) leads to the martensite phase arises inducing strain co-directed with the action of load; the temperature increase in the range $A_s' < T^* < A_f$ causes the recovery of the strain. Therefore, PT-induced strain develops at a given instant and in a given direction $\vec{\mathbf{N}}$ if

$$\dot{\varphi}_N > 0 \text{ for } \dot{T}^* < 0 \left(M_f' < T^* < M_s \right), \tag{10}$$

$$\dot{\varphi}_N < 0 \text{ for } \dot{T}^* > 0 \left(A_s' < T^* < A_f \right), \tag{11}$$

where $\dot{\varphi}_N$ is determined by Eq. (6) whose right-hand side can have different signs different directions $\vec{\mathbf{N}}$. If the sign of function $\dot{\varphi}_N$ from Eq. (6) does not satisfy the condition (10) or (11) for some directions, the phase deformation does not acquire an increment in these directions at the given instant.

There are also other differences between the determination of irreversible strain due to load [2] and phase transitions:

1. A dislocation shape change is neglected due to a PT-induced deformation occurs under stresses below the yield limit.

2. In terms of the synthetic model applied to the description of PTs, there is no concept of yield/creep surface. Therefore, planes, which capable of producing shape changes, fill completely the Ilyushin three-dimensional subspace. Any plane is set by its normal vector $\vec{\mathbf{m}}$ (by angles α and β) and the distance between the plane and the origin of coordinates is characterized by angle λ; $\lambda = 0$ and $\lambda = \pi/2$ give the plane with zero and infinitely large distance, respectively.

3. Planes do not move, i.e. the requirement that a tangent plane produces irreversible strain if only it moves on the endpoint of stress vector is not valid.

4. We do not take into account creep deformation either because loading, unloading, and heating/cooling of body last relatively short time.

4   Modelling of Pseudo-Elatic Strain [4]

Consider the following procedure. A load-free fully austenitic sample is under temperature T_0, $M_s < T_0$. Further, holding the temperature T_0 constant, the specimen is subjected to any proportional loading. Let us consider the case when a thin-walled pipe is subjected to torsion $\left(S_3 = \sqrt{2}\,\tau_{xz} > 0\right)$ and we wish to determine the PT-induced deformation of the pipe. Eq. (2) gives the effective temperature T^* as

$$T^* = T_0\left(1 - D_1 \vec{\mathbf{S}} \cdot \vec{\mathbf{N}}\right). \tag{12}$$

In torsion, we have

$$\vec{\mathbf{S}} \cdot \vec{\mathbf{N}} = S_3 \cos\xi, \quad \cos\xi = \sin\beta\cos\lambda. \tag{13}$$

Hence, Eqs. (12) and (13) give that

$$T^* = T_0\left(1 - D_1 S_3 \cos\xi\right), \tag{14}$$

meaning that the loading of body at constant temperature is equivalent to the decrease in effective temperature, and this reduction varies from plane to plane with different values of angles $\beta > 0$ and λ. T^* is smallest for the plane with $\beta = \pi/2$ and $\lambda = 0$:

$$T^*_{\min} = T_0\left(1 - D_1 S_3\right). \tag{15}$$

If $T^*_{\min}$ decrease to the value of M_s, the martensite phase starts to growth in the plane with $\beta = \pi/2$ and $\lambda = 0$. Equating $T^*_{\min}$ to M_s, we obtain the equation for the stress inducing pseudo-elastic strain – phase flow limit S_Φ (σ_Φ in Fig. 1)– as:

$$S_\Phi = \frac{1}{D_1}\left(1 - \frac{M_s}{T_0}\right). \tag{16}$$

As seen from the above formula, the phase flow limit grows with the temperature of body T_0. If $T_0 = M_s$, $S_\Phi = 0$ and the diagram in Fig. 1 becomes nonlinear at once from the origin of coordinates. The further increase in component S_3 leads to that the effective temperature becomes smaller than M_s meaning the martensitic phase starts to form. The formation of martensite induces strain whose intensity $\dot{\phi}_N$ is determined by Eqs. (6) and (13) as

$$r\dot{\varphi}_N = D_1 T_0 \dot{S}_3 \cos\xi \,. \tag{17}$$

As seen from (17), the conditions (10), $\dot{\varphi}_N \geq 0$, is satisfied for $0 < \lambda < \pi/2$ and $0 < \beta < \pi/2$. On the other hand, the inequality $T^* \leq M_s$ requires

$$\frac{1}{S_3 D_1}\left(1 - \frac{M_s}{T_0}\right) \leq \cos\xi \leq 1 \,, \tag{18}$$

that is obtained by equating T^* to M_s in Eq. (14). With account of (16), the above inequality can be rewritten as $(S_\Phi/S_3) \leq \cos\xi \leq 1$. Therefore, the integration limits in (9) are $0 \leq \alpha \leq 2\pi$, $\beta_1 \leq \beta \leq \pi/2$ and $0 \leq \lambda \leq \lambda_1$:

$$\cos\lambda_1 = S_\Phi/(S_3 \sin\beta) = \sin\beta_1/\sin\beta \,, \quad \sin\beta_1 = S_\Phi/S_3 \,. \tag{19}$$

The macro-strain rate vector components induced by the martensite transformation ($\dot{e}_i^\Phi$), by making use of Eq. (9) are

$$\dot{e}_i^\Phi = \frac{D_1 T_0 \dot{S}_3}{2r} \int_0^{2\pi} d\alpha \int_{\beta_1}^{\pi/2} m_i \sin 2\beta \, d\beta \int_0^{\lambda_1} \cos^2\lambda \, d\lambda \,. \tag{20}$$

Integrating in Eq. (20) gives that $\dot{e}_1^\Phi = \dot{e}_2^\Phi = 0$ and $\dot{e}_3^\Phi$ is

$$\dot{e}_3^\Phi = \frac{2\pi D_1 T_0 \dot{S}_3}{r} \int_{\beta_1}^{\pi/2} \sin^2\beta \cos\beta \, d\beta \int_0^{\lambda_1} \cos^2\lambda \, d\lambda = \frac{\pi D_1 T_0}{3r} Z_1\left(\frac{S_\Phi}{S_3}\right) \dot{S}_3 \,, \tag{21}$$

$$Z_1(x) = \arccos x + x\sqrt{1-x^2} - 2x^3 \ln \frac{1+\sqrt{1-x^2}}{x} \,. \tag{22}$$

Further we integrate over S_3 in limits from S_Φ to S_3 in (21):

$$e_3^\Phi = \frac{\pi D_1 T_0}{3r} \int_{S_\Phi}^{S_3} Z_1\left(\frac{S_\Phi}{S_3}\right) dS_3 = \frac{\pi D_1 T_0 S_\Phi}{3r} F\left(\frac{S_\Phi}{S_3}\right), \tag{23}$$

$$F(x) = \frac{\arccos x}{x} - 2\sqrt{1-x^2} + x^2 \ln \frac{1+\sqrt{1-x^2}}{x} \,.$$

According to Eqs. (7) and (16), we rewrite Eq. (23) as

$$e_3^{\Phi} = \frac{\pi A_f D(T_0 - M_s)}{3(M_s - M_f')} F\left(\frac{S_\Phi}{S_3}\right). \tag{24}$$

This formula holds if the effective temperature (14) less than M_f', i.e. the martensite transformation progresses. Otherwise, according to Fig. 2, the direct martensite transformation is finished ($\Phi = 1$) at $T^* = M_f'$ and, consequently, the transformation-induced deformation is terminated. Equating the right-hand side of Eq. (15) to M_f', we obtain the equation for the boundary value of S_3, S_f, at which Eq. (14) or (15) is applicable:

$$S_\Phi \le S_3 \le S_f \qquad S_f = \frac{1}{D_1}\left(1 - \frac{M_f'}{T_0}\right). \tag{25}$$

Eq. (23) can be obtained in another, simpler, way. By integrating in Eq. (17) with respect to time, we obtain

$$r\varphi_N = D_1 T_0 \cos\xi (S_3 - C), \tag{26}$$

where $C = S_\Phi/\cos\xi$. Therefore,

$$r\varphi_N = D_1 T_0 (S_3 \cos\xi - S_\Phi) = D_1 T_0 S_\Phi\left(\frac{\sin\beta\cos\lambda}{\sin\beta_1} - 1\right). \tag{27}$$

If to insert this strain intensity into Eq. (9) and integrate it, we arrive at the result of Eq. (23).

Somewhat different approach to the modeling of PT-strain can be found in works [5-7].

Conclusions

Utilising the synthetic theory, the phenomenon of pseudo-elasticity has been modelled. To do this the PT-induced lattice distortion D_{ij} and martensitic transformation rate $\dot{\Phi}$ is introduced into the constitutive equtions.

Acknowledgement

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