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Energy Conversion in Shape Memory Alloy Heat Engine Part I: Theory

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ABSTRACT: Shape Memory Alloy (SMA) can be easily deformed to a new shape by applying a small external load at low temperature, and then recovers its original configuration upon heating. This unique shape memory phenomenon has inspired many novel designs. SMA based heat engine is one among them. SMA heat engine is an environment-friendly alternative to extract mechanical energy from low-grade energies, for instance, warm wastewater, geothermal energy, solar thermal energy, etc. The aim of this paper is to present an applicable theoretical model for simulation of SMA-based heat engines. First, a micro-mechanical constitutive model is derived for SMAs. The volume fractions of austenite and martensite variants are chosen as internal variables to describe the evolution of microstructure in SMA upon phase transition. Subsequently, the energy equation is derived based on the first thermodynamic law and the previous SMA model. From Fourier's law of heat conduction and Newton's law of cooling, both differential and integral forms of energy conversion equation are obtained.

INTRODUCTION

A Shape Memory Alloy (SMA) is able to return to a preset shape even after severally deformed. This unique property has attracted a lot of attention since it was found. Many potential applications have been proposed (Funakubo, 1987; Duerig et al., 1990). Some of them are currently available in the market, some are still under investigation, and many more are expected to come very soon.

SMA-based heat engines have been investigated for some years. They are based on the principle that SMAs generate significant force upon temperature change. They can be used as an environment-friendly alternative to extract mechanical energy from low-grade energies, for instance, warm wastewater, geothermal energy, solar thermal energy, etc.

The reported SMA heat engines in the literature are based on various operation principles. Roughly, we may divide them into four categories, namely, offset crank engines, turbine engines, field engines, and miscellaneous (Funakubo, 1987). Spring, wire and rod (including bending rod) are typical shapes of SMAs used. While spring and bending rod can provide far larger

deformation than that of wire and tension rod, the force produced is significantly smaller.

Literature survey shows that the prototypes can run at a speed from 60 rpm to 1000 rpm (Funakubo, 1987; Iwanaga et al., 1988; Gilbertson, 2000). Depending on size, the output power may vary from 0.2 Watt to a few Watts and up to 32 Watts at the most. It is also found that the efficiency of the prototypes may be an order of magnitude below the analytical result (Funakubo, 1987). The significant difference is mainly due to two reasons. One is the use of some very over-optimistic assumptions, and the other is due to the lack of a suitable constitutive model for SMAs. It turns out that an investigation on SMA heat engine using a good model is really necessary.

The aim of this paper is to propose an applicable model for theoretical investigation of SMA-based heat engines. In the second section a constitutive model is derived for SMAs. The third section presents the energy conversion and heat conduction equation of heat engine. The fourth section is conclusions.

CONSTITUTIVE MODEL FOR SMAS

The investigation of SMA based heat engine requires a suitable constitutive model for SMAs. In this section, we present a micro-mechanical model, and then simplify it in order to be applicable in real application.

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Micro-Mechanical Model

Consider a polycrystalline SMA at a temperature higher than austenite finish temperature, A_f . Assume that the whole material is austenite. Refer to Figure 1, consider a Representative Volume Element (RVE) (with volume V and boundary S), which consists of many grains. All grains in this RVE can be divided into N categories according to their grain orientation. The total volume fraction of grains with orientation i is given by c_i .

In martensite, there are n possible Lattice Correspondence Variants (LCVs). Corresponding to a given grain orientation i , the martensite may be divided into n groups based on LCV. Assume the volume fraction of k th group (with orientation i) is z_{ik} and its phase transformation eigenstrain is \mathbf{E}_{ik}^{tr} . Note that $k=0$ represents austenite, in which $\mathbf{E}_{i0}^{tr}=0$.

Suppose that approximately the total local strain \mathbf{e} may be expressed as

$$\mathbf{e} = \mathbf{e}^e + \boldsymbol{\varepsilon}^{tr} \quad (1)$$

where \mathbf{e}^e and $\boldsymbol{\varepsilon}^{tr}$ are elastic strain and phase transformation strain, respectively, and

$$\boldsymbol{\varepsilon}^{tr} = \begin{cases} \mathbf{E}_{ik}^{tr} & (k\text{th group of martensite with orientation } i) \\ 0 & (\text{austenite}) \end{cases} \quad (2)$$

Assume that the specific free energy and specific entropy of austenite and martensite at a given reference temperature T_0 are u_0^A , u_0^M , h_0^A , and h_0^M , respectively. Here, superscript 'A' stands for austenite, while 'M' for martensite. For simplicity, it is reasonable to assume that density ρ is a constant, as volume change in phase transformation is small. Suppose the local specific entropy η^M , elastic energy ϕ , and specific internal energy u in martensite may be written as

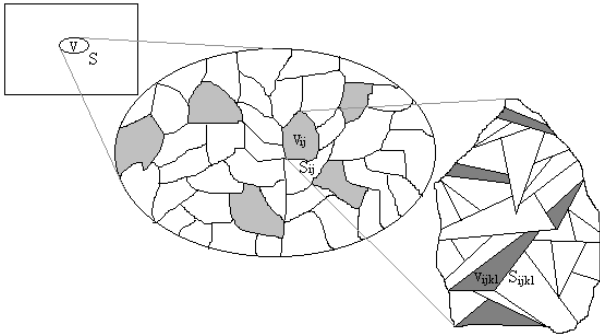


Figure 1. Scale illustration. The gray areas in the middle stand for grains with same orientation in austenite phase. The black areas in the right represent martensite with the same type of lattice corresponding variant.

$$\rho\eta^M(T) = h_0^M + C_V \ln\left(\frac{T}{T_0}\right) \quad (3)$$

$$\phi = \frac{1}{2}(\mathbf{e} - \mathbf{E}_{ik}^{tr}) : \mathbf{L} : (\mathbf{e} - \mathbf{E}_{ik}^{tr}) = \frac{1}{2}\boldsymbol{\sigma} : \mathbf{M} : \boldsymbol{\sigma} \quad (4)$$

$$\rho u = u_0^M + C_V(T - T_0) + \phi \quad (5)$$

where $\boldsymbol{\sigma}$ is local stress, \mathbf{M} elastic compliance tensor, and C_V specific heat. $\mathbf{L} = \mathbf{M}^{-1}$. Symbol “:” stands for double inner product of tensor.

Furthermore, local specific entropy η^A , elastic energy ϕ , and specific internal energy u in austenite may be expressed as

$$\rho\eta^A(T) = h_0^A + C_V \ln\left(\frac{T}{T_0}\right) \quad (6)$$

$$\phi = \frac{1}{2}\mathbf{e} : \mathbf{L} : \mathbf{e} = \frac{1}{2}\boldsymbol{\sigma} : \mathbf{M} : \boldsymbol{\sigma} \quad (7)$$

$$\rho u = u_0^A + C_V(T - T_0) + \phi \quad (8)$$

Hence, given orientation i , $\mathbf{e} = 0$ and $\mathbf{e} = \mathbf{E}_{ik}^{tr}$ ($k = 1, 2, \dots, n$) are $n+1$ potential wells in martensitic transformation.

For any microscopic quantity ψ , its macroscopic quantity may be defined by

$$\langle \psi \rangle = \frac{1}{\rho V} \iiint_V \rho \psi dV \quad (9)$$

In addition, the macroscopic volume average strain is defined by

$$\mathbf{E} = \langle \mathbf{e} \rangle \quad (10)$$

From Equation (1), one has

$$\mathbf{E} = \mathbf{E}^e + \mathbf{E}^{tr} \quad (11)$$

where \mathbf{E}^e and \mathbf{E}^{tr} are macroscopic elastic strain and macroscopic phase transformation strain, respectively, and

$$\mathbf{E}^e = \langle \mathbf{e}^e \rangle \quad (12)$$

$$\mathbf{E}^{tr} = \sum_{i=1}^N c_i \sum_{k=0}^n z_{ik} \mathbf{E}_{ik}^{tr} \quad (13)$$

Similarly, the macro-average of specific entropy ζ , elastic energy Φ and specific internal energy U can be defined as:

$$\zeta = \langle \eta \rangle \quad (14)$$

$$\Phi = \langle \phi \rangle \quad (15)$$

$$U = \langle u \rangle \quad (16)$$

The macroscopic stress applied on volume V is $\boldsymbol{\Sigma}$, where $\boldsymbol{\Sigma}$ is the conjugate stress with macroscopic strain \mathbf{E} , i.e.

$$\frac{1}{V} \iiint_V \boldsymbol{\sigma} : \dot{\mathbf{e}} dV = \boldsymbol{\Sigma} : \dot{\mathbf{E}} \quad (17)$$

Let

$$\dot{W} = \frac{1}{V} \left[\iint_S \boldsymbol{\sigma} : (\mathbf{v} \otimes \mathbf{n}) dA + \iiint_V \mathbf{f} \cdot \mathbf{v} dV \right] \quad (18)$$

where \mathbf{v} is velocity, \mathbf{n} is out normal direction of boundary S , \mathbf{f} is body force. Equations (17) and (18) yield

$$\dot{W} = \frac{1}{V} \iiint_V \boldsymbol{\sigma} : \dot{\mathbf{e}} dV = \boldsymbol{\Sigma} : \dot{\mathbf{E}} \quad (19)$$

The macroscopic Gibbs free energy function is defined by

$$\rho G = \rho U - T \rho \zeta - \boldsymbol{\Sigma} : \mathbf{E} \quad (20)$$

Equations (3)–(8) and (14)–(16) yield

$$\begin{aligned} \rho G = & \sum_{i=1}^N c_i \left[z_{i0}(u_0^A + C_V(T - T_0)) \right. \\ & \left. + \sum_{k=1}^n z_{ik}(u_0^M + C_V(T - T_0)) + f_i^s \right] \\ & - T \left\{ \sum_{i=1}^N c_i z_{i0} \left(h_0^A + C_V \ln \left(\frac{T}{T_0} \right) \right) \right. \\ & \left. + \sum_{k=1}^n z_{ik} \left(h_0^M + C_V \ln \left(\frac{T}{T_0} \right) \right) \right\} \\ & - \boldsymbol{\Sigma} : \left(\sum_{i=1}^N c_i \sum_{k=0}^n z_{ik} \mathbf{E}_{ik}^{tr} \right) - \frac{1}{2} \boldsymbol{\Sigma} : \mathbf{M} : \boldsymbol{\Sigma} \end{aligned} \quad (21)$$

where

$$f_i^s = -\frac{1}{2V_i} \iiint_{V_i} \boldsymbol{\sigma}_{\text{int}} : \boldsymbol{\varepsilon}^{tr} dV \quad (22)$$

Here, V_i is the total volume of grains with orientation i . Let

$$f^s = -\frac{1}{2V} \iiint_V \boldsymbol{\sigma}_{\text{int}} : \boldsymbol{\varepsilon}^{tr} dV \quad (23)$$

Then

$$f^s = \sum_{i=1}^N c_i f_i^s \quad (24)$$

For simplicity, f^s may be taken as the following form,

$$f^s = \sum_{i=1}^N c_i f_i^s = \sum_{i=1}^N c_i A z_{i0} (1 - z_{i0}) \quad (25)$$

Here, A is material constant, and can be measured from experiment. The first thermodynamic law gives,

$$\begin{aligned} \frac{d}{dt} \iiint_V \rho u dV = & \iint_S \boldsymbol{\sigma} : (\mathbf{v} \otimes \mathbf{n}) dA + \iiint_V \mathbf{f} \cdot \mathbf{v} dV \\ & + \iiint_V \rho \dot{r} dV - \iint_S \mathbf{q} \cdot \mathbf{n} dA \end{aligned} \quad (26)$$

Here, \dot{r} is specific heat source and \mathbf{q} is heat flow. Symbol “ \otimes ” stands for tensor product. If the internal specific entropy production is η^* ,

$$\frac{d}{dt} \iiint_V \rho \eta dV = \rho V \eta^* + \iiint_V \frac{1}{T} \rho \dot{r} dV - \iint_S \frac{1}{T} \mathbf{q} \cdot \mathbf{n} dA \quad (27)$$

Provided that temperature T and heat flow \mathbf{q} are uniform in V , using Equation (26), Equation (27) may be rewritten as

$$\begin{aligned} \rho V T \eta^* = & \iint_A \boldsymbol{\sigma} : (\mathbf{v} \otimes \mathbf{n}) dS + \iiint_V \mathbf{f} \cdot \mathbf{v} dV - \frac{d}{dt} \iiint_V \rho u dV \\ & + T \frac{d}{dt} \iiint_V \rho \eta dV - V \frac{1}{T} \mathbf{q} \cdot \nabla T \end{aligned} \quad (28)$$

Using Equations (14), (16) and (18), Equation (28) may be rewritten as

$$\rho T \eta^* = \dot{W} - \rho \dot{U} + \rho T \dot{\zeta} - \frac{1}{T} \nabla T \cdot \mathbf{q} \quad (29)$$

According to Equations (19), (20) and (29), the second thermodynamic law may be written as

$$\begin{aligned} \rho T \eta^* = & -\rho \dot{G} - \rho \zeta \dot{T} - \mathbf{E} : \dot{\boldsymbol{\Sigma}} - \frac{1}{T} \nabla T \cdot \mathbf{q} \\ = & - \left(\mathbf{E} + \rho \frac{\partial G}{\partial \boldsymbol{\Sigma}} \right) : \dot{\boldsymbol{\Sigma}} - \rho \left(\zeta + \frac{\partial G}{\partial T} \right) \dot{T} \\ & - \sum_{i=1}^N c_i \sum_{k=1}^n \rho \frac{\partial G}{\partial z_{ik}} \dot{z}_{ik} - \frac{1}{T} \nabla T \cdot \mathbf{q} \\ \geq & 0 \end{aligned} \quad (30)$$

Therefore

$$\mathbf{E} = -\rho \frac{\partial G}{\partial \boldsymbol{\Sigma}} = \mathbf{M} : \boldsymbol{\Sigma} + \sum_{i=1}^N c_i \sum_{k=1}^n z_{ik} \mathbf{E}_{ik}^{tr} \quad (31)$$

and

$$\zeta = -\frac{\partial G}{\partial T} \quad (32)$$

Let Ξ_{ik} be the thermodynamic driving force corresponding to internal variable z_{ik} ,

$$\Xi_{ik} = -\rho \frac{\partial G}{\partial z_{ik}} = \boldsymbol{\Sigma} : \mathbf{E}_{ik}^{tr} + (\Delta h T - \Delta u) + A(1 - 2z_{i0}) \quad (33)$$

where

$$\left. \begin{aligned} \Delta h &= h_0^M - h_0^A \\ \Delta u &= u_0^M - u_0^A \end{aligned} \right\} \quad (34)$$

Here, Δu is latent heat in phase change, and phase equilibrium temperature $T^{eq} = \Delta u / \Delta h$.

Substituting Equations (31)–(33) into Equation (30) yields

$$\rho T \eta^* = \sum_{i=1}^N c_i \sum_{k=1}^n \Xi_{ik} \dot{z}_{ik} - \frac{1}{T} \nabla T \cdot \mathbf{q} \geq 0 \quad (35)$$

It is well known that Habit Plane Variant (HPV) is not always the minimum sub-unit that composes the bulk martensite. In some SMAs, for instance CuZnAl, HPV is LCV. But in some other SMAs, such as TiNi and CuAlNi, HPV composes two twin-related LCVs (refer to Saburi and Nenno, 1982 for details). Thus, LCV should be potential well instead of HPV. In forward phase transformation, austenite transfers to HPV instead of LCV directly; in reverse transformation, HPV instead of LCV changes back to austenite. Therefore, the relationship between HPV and LCV must be provided. For any given orientation i , introduce volume fraction z_{il}^* for H possible HPVs, which has a direct relation with volume fraction of LCVs as

$$z_{ik} = \sum_{l=1}^H v_{kl} z_{il}^* \quad (k = 0, 1, 2, \dots, n) \quad (36)$$

where v_{kl} is stoichiometric coefficient relating to volume fraction of HPV z_{il}^* .

The phase transformation eigenstrain related to volume fraction z_{il}^* of HPV is

$$\mathbf{E}_{il}^* = \sum_{k=1}^n v_{kl} \mathbf{E}_{ik}^{tr} \quad (37)$$

The thermodynamic driving force corresponding to z_{il}^* is

$$\Pi_{il} = \boldsymbol{\Sigma} : \mathbf{E}_{il}^* + (\Delta h T - \Delta u) + A(1 - 2z_0) \quad (38)$$

Hence, Equation (35) is reduced to

$$\rho T \eta^* = \sum_{i=1}^N c_i \sum_{l=1}^H \Pi_{il} \dot{z}_{il}^* - \frac{1}{T} \mathbf{q} \cdot \nabla T \geq 0 \quad (39)$$

Based on the previous experimental results in, for instance, Huo and Müller (1993); Fu et al. (1993), the critical condition for the start of phase transformation may be expressed as

$$\Pi_{il} = \Pi_{il}^{c\pm}, \quad (l = 1, 2, \dots, H) \quad (40)$$

where “+” corresponds to the forward transformation, and “−” corresponds to the reverse transformation.

$\Pi_{il}^{c+} > 0$ and $\Pi_{il}^{c-} < 0$ correspond to the critical thermodynamic driving forces for forward transformation and reverse transformation, respectively.

The evolution equation for further phase transformation may be expressed as

$$\left. \begin{aligned} \dot{\Pi}_{il} &= \dot{\Pi}_{il}^{c+} = 2 \left(\lambda + \mu \frac{1}{z_{i0}^*} \right) \dot{z}_{il}^* \\ &\quad \text{(for forward transformation)} \\ \dot{\Pi}_{il} &= \dot{\Pi}_{il}^{c-} = 2 \left(\lambda + \mu \frac{1}{z_{il}^*} \right) \dot{z}_{il}^* \\ &\quad \text{(for reverse transformation)} \end{aligned} \right\} \quad (41)$$

Here, λ and μ are non-negative material constants. They are introduced to describe hardening behavior, and can be measured from experiment. For a material with hardening behavior, the following relation is usually observed,

$$\lambda > A \quad (42)$$

In forward transformation, Π_{il}^{c+} increases, while in reverse transformation, Π_{il}^{c-} decreases. In forward transformation, as soon as nucleation starts, Π_{il}^{c-} moves back to its maximum value ($-\Pi_0$). When reverse transformation starts, Π_{il}^{c+} returns to its minimum value (Π_0) instantly. Π_0 is non-negative material constant. From Equations (40) and (41), we can get volume fraction of each HPV. The eigenstrain of phase transformation may be calculated by

$$\mathbf{E}^{tr} = \sum_{i=1}^N c_i \sum_{l=1}^H z_{il}^* \mathbf{E}_{il}^* \quad (43)$$

Simplification

In theory, the model presented above can be use for all kinds of SMAs (single crystal, textured/non-textured polycrystal) under various loading processes, including thermal cycling. But it is too tedious to be applied in a real analysis.

In the case of non-textured SMA, additional assumptions are made here to simplify the model.

- As non-textured polycrystal consists of a lot of randomly and uniformly distributed grains, it is reasonable to say that N orientation groups are uniformly distributed. So the volume fraction of each orientation group is the same, i.e., $c_i = 1/N$ ($i = 1, 2, \dots, N$).
- The interaction among HPVs is small and can be ignored, i.e., $\mu = 0$ in Equation (41). Furthermore, we suppose that the phase transformation mechanism of polycrystal at microscopic level is the same as that of single variant phase transformation in single crystalline material. So each orientation group has

H possible phase transformation systems. They are independent on each other.

Based on assumptions (a) and (b), we may directly divide a RVE into N_0 orientation components, where $N_0 = N \times H$. The volume fraction of each orientation component in this RVE is $1/N_0$.

(c) The small amount of volume change upon phase transformation is ignored. Let martensite volume fraction of orientation component k be z_k , so the volume fraction of austenite is $z_{k0} = 1 - z_k$.

According to assumption (c), Equation (43) may be written as

$$\mathbf{E}^{tr} = \frac{1}{N_0} g \sum_{k=1}^{N_0} z_k \mathbf{P}_k \quad (44)$$

where g is the magnitude of shear of orientation component k , and

$$\mathbf{P}_k = \frac{1}{2}(\mathbf{m}_k \otimes \mathbf{n}_k + \mathbf{n}_k \otimes \mathbf{m}_k) \quad (45)$$

Here, \mathbf{n}_k is normal direction of habit plane of orientation component k , \mathbf{m}_k is shear direction. They are assumed to distribute uniformly on the surface of a unit sphere.

The corresponding shear stress is obtained by

$$\tau_k = \boldsymbol{\Sigma} : \mathbf{P}_k \quad (46)$$

Thus, Equation (38) may be written as

$$\Pi_k = \tau_k g + (\Delta h T - \Delta u) - A(1 - 2z_k) \quad (47)$$

The critical condition for the start of phase transformation becomes,

$$\Pi_k = \Pi_k^{c\pm}, \quad (k = 1, 2, \dots, N_0) \quad (48)$$

And the equation for the evolution of phase transformation becomes,

$$\left. \begin{aligned} \dot{\Pi}_k &= \dot{\Pi}_k^{c+} = 2\lambda \dot{z}_k^* & \text{for forward transformation} \\ \dot{\Pi}_k &= \dot{\Pi}_k^{c-} = 2\lambda \dot{z}_k^* & \text{for reverse transformation} \end{aligned} \right\} \quad (49)$$

If the martensite volume fraction of each orientation component is determined, the total strain can be calculated by

$$\mathbf{E} = \mathbf{M} : \boldsymbol{\Sigma} + \frac{1}{N_0} g \sum_{k=1}^{N_0} z_k \mathbf{P}_k \quad (50)$$

ENERGY CONVERSION

Recall Equation (18), Equation (26) may be rewritten as

$$\nabla \cdot \mathbf{q} - \rho \dot{r} = \dot{W} - \rho \dot{U} \quad (51)$$

From Equations (29) and (35), we have

$$\dot{W} - \rho \dot{U} + T \rho \dot{\xi} = \sum_{i=1}^N c_i \sum_{k=1}^n \Xi_{ik} \dot{z}_{ik} \quad (52)$$

Combining Equations (51) and (52) together, following is obtained,

$$\nabla \cdot \mathbf{q} - \rho \dot{r} = \sum_{i=1}^N c_i \sum_{k=1}^n \Xi_{ik} \dot{z}_{ik} - \rho T \dot{\xi} \quad (53)$$

Equations (3), (6) and (14) yield

$$\begin{aligned} \rho \dot{\xi} &= \sum_{i=1}^N c_i \left[z_{i0} \left(h_0^A + C_V \ln \left(\frac{T}{T_0} \right) \right) \right. \\ &\quad \left. + \sum_{k=1}^n z_{ik} \left(h_0^M + C_V \ln \left(\frac{T}{T_0} \right) \right) \right] \end{aligned} \quad (54)$$

Thus

$$\rho T \dot{\xi} = C_V \dot{T} + \Delta h T \sum_{i=1}^N c_i \sum_{k=1}^n \dot{z}_{ik} \quad (55)$$

Equations (53) and (55) yield

$$C_V \dot{T} = \rho \dot{r} - \nabla \cdot \mathbf{q} + \sum_{i=1}^N c_i \sum_{k=1}^n (\Xi_{ik} - \Delta h T) \dot{z}_{ik} \quad (56)$$

Substituting Equation (33) into Equation (56), and recalling Equations (13) and (25), one has

$$\boldsymbol{\Sigma} : \dot{\mathbf{E}}^{tr} = \nabla \cdot \mathbf{q} - \rho \dot{r} + C_V \dot{T} + \Delta u \dot{z} + \dot{f}^s \quad (57)$$

where the total volume fraction of martensite is

$$z = \sum_{i=1}^N c_i \sum_{k=1}^n z_{ik} \quad (58)$$

Fourier heat conduction equation is given by

$$\mathbf{q} = -k \nabla T \quad (59)$$

where k is thermal conductivity. According to Newton's law of cooling we have

$$k \frac{\partial T}{\partial n} = \alpha (T_W - T) \quad (60)$$

where α is the heat exchange coefficient.

Hence,

$$\iiint_V (-\nabla \cdot \mathbf{q}) dV = \oint_S k \frac{\partial T}{\partial n} dA = \oint_S \alpha (T_W - T) dA \quad (61)$$

Integration of Equation (56) yields

$$\begin{aligned} & \iiint_V \rho \dot{r} dV + \oint_S \alpha (T_W - T) dA \\ & + \iiint_V \left\{ \sum_{i=1}^N c_i \sum_{k=1}^n (\Xi_{ik} - \Delta h T) \dot{z}_{ik} \right\} dV = \iiint_V C_V \dot{T} dV \end{aligned} \quad (62)$$

Rewrite Equation (62) as

$$\begin{aligned} & \iiint_V \rho \dot{r} dV + \oint_S \alpha (T_W - T) dA \\ & + \iiint_V \left\{ \sum_{i=1}^N c_i \sum_{l=1}^H (\Pi_{il} - \Delta h T) \dot{z}_{il}^* \right\} dV \\ & = \iiint_V C_V \dot{T} dV \end{aligned} \quad (63)$$

For simplified model, it turns to be

$$\begin{aligned} & \iiint_V \rho \dot{r} dV + \oint_S \alpha (T_W - T) dA \\ & + \iiint_V \left\{ \frac{1}{N_0} \sum_{k=1}^{N_0} (\Pi_k - \Delta h T) \dot{z}_k \right\} dV \\ & = \iiint_V C_V \dot{T} dV \end{aligned} \quad (64)$$

Integration of Equation (57) results in the final formula, which can be used in real application,

$$\begin{aligned} & \iiint_V (\Sigma : \mathbf{E}^{tr}) dV + \iiint_V \rho \dot{r} dV + \oint_S \alpha (T_W - T) dA \\ & = \iiint_V C_V \dot{T} dV + \iiint_V \Delta u \dot{z} dV + \iiint_V \dot{f}^s dV \end{aligned} \quad (65)$$

CONCLUSIONS

In this paper, we present a theoretical model for simulation of SMA based heat engines. First, we derive a micro-mechanical model for SMAs, and then simplify it to be suitable in real analysis. Subsequently, this simplified model is integrated with the analysis of energy conversion in SMA heat engine. The resulting formula includes six terms. They are 1) work done in phase transformation; 2) contribution from heat resource; 3) total absorbed heat; 4) thermal term related to the temperature change in SMA; 5) latent heat in phase transformation; and 6) stored elastic energy in SMA.

For details of characterization of parameters in this model, readers may refer to Zhu et al. (2001b). This model has been used to simulate the behavior of an actual SMA heat engine. The result appears in Part II of this paper (Zhu et al., 2001a).

REFERENCES

- Duerig, T. W., Melton, K. N., Stoeckel, D. and Wayman, C. M. (1990). *Engineering aspects of shape memory alloys*, Butterworth-Heinemann Ltd.
- Fu, S., Huo, Y. and Müller, I. (1993). Thermodynamics of pseudoelasticity – an analytical approach, *Acta Mech.*, **99**:1–19.
- Funakubo, H. (1987). *Shape memory alloys*, Gordon and Breach Science Publishers.
- Gilbertson, R. G. (2000). *Muscle wires project book*, 3rd edition, Mondo-tronics Inc.
- Huo, Y. and Müller, I. (1993). Nonequilibrium thermodynamics of pseudoelasticity, *Count. Mech. Thermodyn.*, **5**(1):163–204.
- Iwanaga, H., Tobushi, H. and Ito, H. (1988). Basic research on output power characteristics of a shape memory alloy heat engine, *JSME Int. J.*, Series. I, **31**:634–637.
- Saburi, T. and Nenno, S. (1982). The shape memory effect and related phenomena. In: *Proc. Int. Conf. on Solid to Solid Phase Transformation* (eds: Aaronson, H.I. et al.). 1455–1479
- Zhu, J. J., Liang, N. G. Huang, W. M. and Liew, K. M. (2001a). Energy conversion in shape memory alloy heat engine. Part II: Simulation. *J. Intell. Mater. Syst. Struct.* **12**:133–140.
- Zhu, J. J., Liang, N. G. Huang, W. M. Liew, K. M. and Liu, Z. H. (2001b). A thermodynamic constitutive model for stress induced phase transformation in shape memory alloys, *Int. J. Solids Struct.* (in press).